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Table 1: Proton assignment for horse heart ferricytochrome *c* at 293 K
Note: The underlined chemical shifts indicate the stereospecific assignment for diastereotopic pairs of methylene protons or isopropyl methyl groups

residue	HN	HA		HB		others		
1	8.10	3.52	3.80					
2	9.24	4.64		2.66	2.35			
3	8.47	3.45		2.07		0.95(QG1)	0.99(QG2)	
4	8.03	4.03		2.08	2.01	2.29(HG2)	2.22(HG3)	
5	8.04	3.83		1.63		0.86(QG)	2.84(QD)	3.12(QE)
6	8.67	3.88	3.18					
7	7.98	2.20		1.66		1.39(QG)	0.87(QD)	1.13(QE)
8	6.86	3.83		1.78	1.57	1.52(QG)	1.30(QD)	2.87(QE)
9	7.43	3.46		1.54		0.32(QG2)	0.86(QG1)	0.67(QD1)
10	8.36	3.37		3.11	2.68	7.48(HD1)	8.33(HE1)	8.73(HZ)
						7.58(HE2)	6.84(HD2)	
11	8.83	3.81		2.18		1.27(QG1)	1.05(QG2)	
12	7.78	4.09		1.95	2.03	2.22 (HG2)	2.48(HG3)	6.77(NH1)
						7.38(NH2)		
13	8. 43	4.31		1.10		0.77(QG)	3.15(QE)	
14	8.04	4.31						
15	8.09	5.96		2.17				
16	9.89	4.75		2.39	2.61	2.95 (HG2)	2.79(HG3)	6.90(NH1)
						7.61(NH2)		
17	9.63	5.99		2.07	7.07			
18	10.94	9.10		8.94	14.70	12.80(HD1)	24.71(HD2)	-25.67(HE1)
19	10.69	6.24		5.54		2.19(QG2)	8.98(OH)	
20	8.89	4.99		2.18		0.97(QG1)	1.01(QG2)	
21	9.59	4.63		2.51				
22	9.09	3.35		1.49	0.94	0.70(QG)	1.11(QD)	2.91(QE)
23	9.42	3.72	4.04					
24	8.22	3.67	4.29					
25	8.81	4.21		2.01	1.86	1.64(HG2)	1.59(HG3)	1.77(QD)
						3.07(QE)		
26	8.85	5.01		3.04	2.69	6.91(HD2)	7.58(HE1)	
27	8.32	4.63		1.47				
28	7.92	3.00		2.99		-0.13(QG2)		
29	6.91	-1.09	-4.43					
30		3.70		1.32	1.40	-1.11(HG2)	-0.42(HG3)	-2.45(HD2)
						-6.64(HD3)		
31	11.56	5.94		2.88	2.50			
32	9.59	4.99		2.58		2.32(HG)	2.05(QD1)	1.66(QD2)
33	8.33	4.27		3.30				
34	9.02	3.78	4.01					
35	7.07	3.58		2.16	1.42	1.04(HG)	0.43(QD1)	0.10(QD2)
36	8.63	3.75		2.71	3.16	7.19(CG)	6.54(CZ)	6.69(HZ)
37	9.28	4.33	3.42					
38	8.16	4.60		2.09	1.85	2.02(QG)	3.14(QD)	
39	8.02	4.85		1.62	1.55	1.28(QG)		
40	7.53	4.12		4.43		0.79(QG2)	7.29(OH)	

41	9.14	1.16	3.00					
42	7.70	4.37		2.42	1.61	2.12(HG2) 7.41(NH2)	2.03(HG3)	6.87(NH1)
43	8.03	4.56		1.41				
44		4.37		1.99	2.30	2.24(HG1)	2.01(HG3)	3.82(HD2)
45	8.95	3.64	4.37					
46	6.81	3.63		1.71	0.58	5.68(HD1) 4.89(HE2)	5.44(HE1) 3.65(HD2)	4.68(HZ)
47	6.72	3.73		3.09		0.64(QG2)		
48	7.97	4.02		3.06	2.35	6.92(CG)	5.56(CZ)	
49	9.59	4.10		4.79		1.47(QG2)		
50	8.85	4.20		2.57				
51	8.06	4.13		1.60				
52	8.54	4.67		3.17	3.05			
53	8.64	3.69		1.82		1.37(QG)	1.74(QD)	2.90(QE)
54	8.16	4.79		2.90	2.70	6.99(NH1)	7.43(NH2)	
55	6.99	4.22		1.83	2.18	1.63(QG)	1.76(QD)	3.06(QE)
56	7.83	3.81	3.70					
57	6.53	4.44		1.85		1.15(HG12) -0.44(QD1)	0.63(HG13)	0.78(QG2)
58	8.26	4.12		3.71		0.88(QG2)	8.16(OH)	
59	8.71	4.68		3.58	2.03	6.80(HD1) 6.45(HZ3)	7.28(HE3) 7.53(HZ2)	9.52(HE1) 6.28(HH2)
60	7.95	4.22		1.95		1.37(QG)	1.55(QD)	2.29(QE)
61	10.66	3.59		2.05		2.45(QG)		
62	9.50	3.93		2.01	1.95	2.29(HG2)	2.35(HG3)	
63	7.01	4.31		4.50		1.33(QG2)		
64	8.48	3.76		1.50	0.38	1.25(HG)	-0.66(QD1)	-0.30(QD2)
65	8.21	3.60		2.05	1.95			
66	6.59	4.05		1.95	1.72	2.08(HG2)	2.37(HG3)	
67	8.06	3.93		3.25	2.60			
68	8.08	2.53		0.92	-0.14	0.58(HG)	-2.88(QD1)	-0.70(QD2)
69	6.76	3.80		2.04	2.09			
70	6.65	4.78		3.18	3.10			
71		5.38				3.24(HG2) 3.63(HD3)	2.05(HG3)	4.28(HD2)
72	9.45	5.23		2.60	2.76	2.32(HG2)	3.55(HG3)	
73	7.79	4.44		2.02	2.07	1.64(QG)	1.86(QD)	3.14(QE)
74	8.10			1.90		7.70(CG)	6.75(CZ)	
75	9.46	4.92		3.45		1.29(QG2)	2.03(QD1)	
76		5.19		2.58	2.09	2.27(HG2)	3.70HG3)	3.79(QD)
77	9.36	4.57	4.00					
78	9.04	5.20		5.92		3.51(QG2)	9.57(OH)	
79	8.23					0.72(HG2)	0.38(HG3)	2.29(QE)
80	9.25	2.77		12.79	7.60	-28.57 (HG)	-24.83(QE)	
81	8.57	5.10		2.10		1.08(QG2) 0.90(QD1)	1.37(HG12)	1.56(HG13)
82	9.01	4.53		3.64		6.00(CG)	5.96(CZ)	5.81(HZ)
83	8.49	4.23		1.22				
84	8.43	2.65	4.31					
85	7.96	3.80		0.77		0.49(QG2) -0.29(QD1)	0.57(HG12)	0.32(HG13)

86	8.42	3.90	1.71	1.63	1.38(QG) 2.88(HE3)	1.54(QD)	2.81(HE2)
87	8.20	4.10	1.48				
88	8.93	3.44	1.72		0.52(QG)	1.16(QD)	1.51(QE)
89	8.11	3.89	3.99		1.16(QG2)		
90	6.02	3.93	1.68	1.53	2.03(QG)		
91	7.08	3.15	1.82	1.66			
92	8.22	3.51	2.20	2.50(QG)			
93	8.21	3.99	2.37				
94	7.88	3.74	1.38	1.01	0.61(HG)	0.52(QD1)	-0.38(QD2)
95	8.39	3.01	1.58		0.39(QG2) 0.17(QD1)	1.22(HG12)	0.78(HG13)
96	7.79	3.89	1.19				
97	7.88	4.09	2.77	3.47	6.33(HD1) 7.07(HD2)	5.65(HE1)	6.77(HE2)
98	8.71	3.31	1.77	0.98	1.57(HG)	0.41(QD1)	-0.22(QD2)
99	8.83	2.42	1.44		0.68(QG) 2.58(HE3)	0.11(QD)	2.62(HE2)
100	6.73	4.00	1.66	1.71	1.19(HG2)	1.33(HG3)	2.97(QE)
101	8.63	4.00	0.72				
102	7.92	4.55			1.23(QG2)	6.42(OH)	
103	7.10	4.93	2.80	2.53			
104	7.38	4.27	2.04		2.34(QG)		

Heme-protons:

35.74(QM8) 2.10(HDM) 6.81(QM1) -1.33(HT2A) -2.63(QT2) 1.40(HAM)
32.77(QM3) 2.09(HT4A) 3.05(QT4) -0.92(HBM) 9.72(QM5) 7.51(HGM)
11.38(HAP71) 19.23(HAP72) 1.57(HBP73) -0.44(HBP74) -1.55(HAP61) 1.68(HAP62)

Table 2: Experimental NOE intensities

1 GLY			
	HN	1 GLY HA1	11990.0 e
	HN	1 GLY HA2	18210.0 e
	HN	2 ASP- HN	2737.0 e
	HN	86 LYS+ HE3	376.0 e
	HN	96 ALA QB	8530.0 e
	HA1	2 ASP- HN	19890.0 e
	HA1	93 ASP- HA	21800.0 e
	HA1	96 ALA HA	1680.0 e
	HA1	96 ALA QB	24300.0 e
	HA2	2 ASP- HN	16560.0 e
	HA2	93 ASP- HN	2821.0 e
	HA2	96 ALA QB	9389.0 e
2 ASP-			
	HN	2 ASP- HA	532.0 e
	HN	2 ASP- HB2	15700.0 e
	HN	2 ASP- HB3	11950.0 e
	HN	3 VAL HN	293.0 e
	HN	5 LYS+ HN	395.0 e
	HN	5 LYS+ QB	1195.5*2e
	HN	5 LYS+ QD	412.0*2e
	HN	6 GLY HN	207.0 e
	HN	93 ASP- HA	5063.0 e
	HN	96 ALA HN	434.0 e
	HN	96 ALA HA	870.0 e
	HN	96 ALA QB	6398.0 e
	HA	3 VAL HN	5118.0 e
	HA	3 VAL QG1	2741.0 e
	HA	3 VAL QG2	776.0 e
	HB2	3 VAL HN	292.0 e
	HB2	3 VAL HA	1231.0 e
	HB2	5 LYS+ HN	5562.0 e
	HB2	5 LYS+ QB	2280.5*2e
	HB2	6 GLY HN	255.0 e
	HB3	3 VAL HN	474.0 e
	HB3	3 VAL QG1	2130.0 e
	HB3	3 VAL QG2	1602.0 e
	HB3	4 GLU- HN	1058.0 e
	HB3	5 LYS+ HA	580.0 e
	HB3	6 GLY HN	1514.0 e
3 VAL			
	HN	3 VAL HA	8426.0 e
	HN	3 VAL HB	10960.0 e
	HN	3 VAL QG1	24150.0 e
	HN	3 VAL QG2	11400.0 e
	HN	4 GLU- HN	28230.0 e
	HN	4 GLU- HA	87.0 e
	HN	96 ALA QB	6310.0 e
	HA	3 VAL HB	18660.0 e
	HA	3 VAL QG1	30940.0 e
	HA	3 VAL QG2	26980.0 e
	HA	4 GLU- HN	4330.0 e
	HA	4 GLU- HA	452.0 e
	HA	6 GLY HN	2480.0 e
	HA	6 GLY HA1	145.0 e
	HA	7 LYS+ HN	1968.0 e
	HA	96 ALA QB	8736.0 e
	HB	3 VAL QG1	75630.0 e
	HB	3 VAL QG2	82550.0 e
	QG1	4 GLU- HN	7117.0 e
	QG1	4 GLU- HA	2868.0 e
	QG1	7 LYS+ QB	9840.0*2e
	QG1	96 ALA HA	629.0 e
	QG1	97 TYR HD1	1744.0 e
	QG1	100 LYS+ QE	1926.5*2e
	QG2	4 GLU- HN	4933.0 e
	QG2	4 GLU- HA	4927.0 e
	QG2	7 LYS+ HN	651.0 e
	QG2	7 LYS+ QB	10185.0*2e
	QG2	96 ALA HN	2552.0 e
	QG2	96 ALA HA	815.0 e
	QG2	97 TYR HA	39600.0 e
	QG2	100 LYS+ QE	1907.5*2e
4 GLU-			
	HN	4 GLU- HA	16260.0 e
	HN	4 GLU- HB2	30210.0 e
	HN	4 GLU- HB3	27920.0 e
	HN	4 GLU- HG2	5844.0 e
	HN	4 GLU- HG3	10940.0 e
	HN	6 GLY HN	5681.0 e
	HA	4 GLU- HB2	13920.0 e
	HA	4 GLU- HB3	21990.0 e
	HA	4 GLU- HG2	11120.0 e
	HA	4 GLU- HG3	11570.0 e
	HA	5 LYS+ HN	1597.0 e
	HA	7 LYS+ HN	3889.0 e
	HA	7 LYS+ QB	2870.5*2e
	HA	7 LYS+ QG	1076.0*2e
	HA	7 LYS+ QD	163.5*2e
5 LYS+			
	HN	5 LYS+ HA	9868.0 e
	HN	5 LYS+ QB	9205.0*2e
	HN	5 LYS+ QD	173.0*2e
	HN	6 GLY HN	4942.0 e
	HN	93 ASP- QB	235.0*2e
	HA	5 LYS+ QB	15115.0*2e
	HA	5 LYS+ QG	606.0*2e
	HA	5 LYS+ QD	1813.0*2e
	HA	6 GLY HN	2791.0 e
	QB	5 LYS+ QG	14260.0*4e
	QB	6 GLY HN	5805.0*2e
	QB	6 GLY HA2	3862.0*2e
	QD	5 LYS+ QE	58.5*4e
	QE	9 ILE QD1	961.5*2e
6 GLY			
	HN	6 GLY HA1	5057.0 e
	HN	6 GLY HA2	9553.0 e
	HN	7 LYS+ HN	4863.0 e
	HN	8 LYS+ HN	427.0 e
	HN	9 ILE HN	62.0 e
	HN	9 ILE QG2	59.0 e
	HN	9 ILE QG1	351.0*2e
	HN	93 ASP- QB	1676.5*2e
	HN	96 ALA QB	1754.0 e
	HA1	7 LYS+ HN	1157.0 e
	HA1	8 LYS+ HN	667.0 e
	HA1	9 ILE HN	6736.0 e
	HA1	9 ILE QG2	2436.0 e
	HA1	9 ILE QG1	480.5*2e

HA1	9 ILE QD1	10220.0	e
HA1	93 ASP- QB	856.0*2	e
HA2	7 LYS+ HN	4202.0	e
HA2	7 LYS+ HA	1782.0	e
HA2	8 LYS+ HN	519.0	e
HA2	9 ILE HB	2634.0	e
HA2	9 ILE QD1	4648.0	e
HA2	10 PHE HN	964.0	e
HA2	97 TYR HB2	863.0	e

7 LYS+

HN	7 LYS+ HA	11630.0	e
HN	7 LYS+ QB	5925.0*2	e
HN	7 LYS+ QG	3139.0*2	e
HN	7 LYS+ QD	644.5*2	e
HN	8 LYS+ HN	8905.0	e
HN	97 TYR HA	355.0	e
HN	97 TYR HB2	1720.0	e
HN	97 TYR HB3	424.0	e
HN	97 TYR HD1	524.0	e
HN	97 TYR HD2	1454.0	e
HA	8 LYS+ HN	4410.0	e
HA	97 TYR HB2	4325.0	e
HA	97 TYR HD2	5739.0	e
QB	8 LYS+ HN	3757.0*2	e
QG	8 LYS+ HN	3351.0*2	e
QG	97 TYR HE1	968.5*2	e
QD	8 LYS+ HN	612.0*2	e
QD	97 TYR HD1	342.0*2	e
QD	97 TYR HD2	97.5*2	e
QD	97 TYR HE1	1888.5*2	e
QD	97 TYR HE2	648.0*2	e

8 LYS+

HN	8 LYS+ HA	22140.0	e
HN	8 LYS+ HB2	43870.0	e
HN	8 LYS+ HB3	9420.0	e
HN	8 LYS+ QG	9110.0*2	e
HN	8 LYS+ QD	4958.5*2	e
HN	8 LYS+ QE	926.0*2	e
HN	9 ILE HN	15850.0	e
HN	9 ILE HA	622.0	e
HN	9 ILE QG1	890.0*2	e
HN	9 ILE QD1	104.0	e
HN	11 VAL QG1	2474.0	e
HA	8 LYS+ HB2	80140.0	e
HA	8 LYS+ HB3	21700.0	e
HA	8 LYS+ QG	9450.0*2	e
HA	8 LYS+ QD	6295.0*2	e
HA	8 LYS+ QE	2744.5*2	e
HA	9 ILE HN	7128.0	e
HA	10 PHE HN	1582.0	e
HB2	8 LYS+ QD	31855.0*2	e
HB2	8 LYS+ QE	8985.0*2	e
HB2	9 ILE HN	11160.0	e
HB2	12 GLN HN	151.0	e
QD	8 LYS+ QE	4085.0*4	e
QE	12 GLN HE22	418.5*2	e
QE	97 TYR HE2	400.5*2	e

9 ILE

HN	9 ILE HA	12740.0	e
HN	9 ILE HB	45620.0	e
HN	9 ILE QG2	10400.0	e
HN	9 ILE QG1	6750.0*2	e
HN	9 ILE QD1	9939.0	e
HN	10 PHE HN	25920.0	e
HN	10 PHE HA	1418.0	e
HN	11 VAL HN	4915.0	e
HN	12 GLN HG3	180.0	e
HN	13 LYS+ HN	657.0	e
HA	9 ILE HB	20730.0	e
HA	9 ILE QG2	39430.0	e
HA	9 ILE QG1	11420.0*2	e
HA	9 ILE QD1	10090.0	e
HA	10 PHE HN	5532.0	e
HA	12 GLN HN	4859.0	e
HA	13 LYS+ HN	949.0	e
HB	9 ILE QG2	42930.0	e
HB	9 ILE QG1	36635.0*2	e
HB	9 ILE QD1	75250.0	e
HB	10 PHE HN	5780.0	e
QG2	9 ILE QG1	17335.0*2	e
QG2	9 ILE QD1	61740.0	e
QG2	10 PHE HN	6380.0	e
QG2	10 PHE HA	4117.0	e
QG2	10 PHE HD1	906.0	e
QG2	12 GLN HN	931.0	e
QG2	13 LYS+ QE	549.0*2	e
QG2	94 LEU HN	1957.0	e
QG2	94 LEU HA	1723.0	e
QG2	94 LEU HB3	26740.0	e
QG2	94 LEU QD2	23550.0	e
QG1	9 ILE QD1	27255.0*2	e
QG1	10 PHE HN	474.0*2	e
QD1	10 PHE HN	3479.0	e
QD1	18 HEM QT2	809.0	e
QD1	90 GLU- HA	14400.0	e
QD1	93 ASP- QB	5145.0*2	e
QD1	94 LEU HN	4369.0	e
QD1	94 LEU HA	4986.0	e

10 PHE

HN	10 PHE HA	21730.0	e
HN	10 PHE HB2	30320.0	e
HN	10 PHE HB3	27940.0	e
HN	11 VAL HN	14300.0	e
HN	11 VAL HA	358.0	e
HN	11 VAL QG1	1375.0	e
HN	18 HEM QT2	472.0	e
HN	94 LEU QD1	19340.0	e
HN	97 TYR HB2	1486.0	e
HN	97 TYR HD1	3074.0	e
HN	97 TYR HD2	611.0	e
HN	97 TYR HE1	4103.0	e
HA	10 PHE HB2	25370.0	e
HA	10 PHE HB3	28480.0	e
HA	10 PHE HD1	3197.0	e
HA	10 PHE HD2	13280.0	e
HA	11 VAL HN	3447.0	e
HA	11 VAL HA	2166.0	e
HA	13 LYS+ HN	2331.0	e
HA	14 CYSS HN	2501.0	e
HA	18 HEM QT2	2540.0	e
HA	94 LEU QD1	15960.0	e
HA	94 LEU QD2	2375.0	e
HA	97 TYR HD1	1397.0	e
HA	97 TYR HE1	644.0	e

HB2 10 PHE HD1 9861.0 e
HB2 10 PHE HD2 17740.0 e
HB2 11 VAL HN 5134.0 e
HB2 94 LEU QD1 11000.0 e
HB2 97 TYR HD1 3791.0 e
HB2 97 TYR HE1 5831.0 e
HB2 98 LEU QD1 653.0 e
HB3 10 PHE HD1 15650.0 e
HB3 10 PHE HD2 19070.0 e
HB3 11 VAL HN 1209.0 e
HB3 94 LEU QD1 7406.0 e
HB3 94 LEU QD2 1104.0 e
HB3 97 TYR HD1 5652.0 e
HB3 97 TYR HE1 4860.0 e
HD1 10 PHE HE1 27500.0 e
HD1 10 PHE HE2 15890.0 e
HD1 10 PHE HZ 4821.0 e
HD1 11 VAL HN 3554.0 e
HD1 11 VAL HB 3540.0 e
HD1 11 VAL QG1 915.0 e
HD1 11 VAL QG2 436.0 e
HD1 18 HEM HB3 524.0 e
HD1 20 VAL QG1 509.0 e
HD1 97 TYR HD1 2108.0 e
HD1 97 TYR HE1 2891.0 e
HD1 98 LEU QD2 7782.0 e
HD2 10 PHE HE1 38240.0 e
HD2 10 PHE HE2 19540.0 e
HD2 10 PHE HZ 8845.0 e
HD2 11 VAL HN 1728.0 e
HD2 11 VAL HA 3257.0 e
HD2 11 VAL QG1 4600.0 e
HD2 11 VAL QG2 1228.0 e
HD2 15 ALA HA 833.0 e
HD2 18 HEM QT2 243.0 e
HD2 20 VAL QG1 359.0 e
HD2 94 LEU QD1 17200.0 e
HD2 94 LEU QD2 2497.0 e
HD2 97 TYR HD1 619.0 e
HD2 97 TYR HE1 2648.0 e
HD2 98 LEU QD1 1605.0 e
HD2 98 LEU QD2 11110.0 e
HE1 10 PHE HZ 44420.0 e
HE1 11 VAL QG1 1340.0 e
HE1 11 VAL QG2 681.0 e
HE1 15 ALA HA 5204.0 e
HE1 15 ALA QB 9499.0 e
HE1 18 HEM HN 590.0 e
HE1 18 HEM HB2 745.0 e
HE1 18 HEM HB3 3097.0 e
HE1 19 THR HA 1534.0 e
HE1 20 VAL QG1 6453.0 e
HE1 98 LEU QD1 349.0 e
HE1 98 LEU QD2 4886.0 e
HE1 101 ALA QB 554.0 e
HE2 10 PHE HZ 32320.0 e
HE2 15 ALA HA 1954.0 e
HE2 15 ALA QB 5049.0 e
HE2 18 HEM HB2 1391.0 e
HE2 18 HEM HB3 3804.5 e
HE2 20 VAL QG1 3653.0 e
HE2 32 LEU QD2 880.0 e
HE2 97 TYR HE1 1212.0 e
HE2 98 LEU QD1 1254.0 e
HE2 98 LEU QD2 8714.0 e
HZ 15 ALA HA 5630.0 e
HZ 15 ALA QB 4429.0 e
HZ 18 HEM HN 1442.0 e
HZ 18 HEM HB2 8292.0 e
HZ 18 HEM HB3 20080.0 e
HZ 19 THR HN 1781.0 e
HZ 19 THR HA 6615.0 e
HZ 19 THR HB 469.0 e
HZ 20 VAL QG1 15720.0 e
HZ 32 LEU QD1 3645.0 e

11 VAL
HN 11 VAL HA 18110.0 e
HN 11 VAL HB 20180.0 e
HN 11 VAL QG1 34620.0 e
HN 11 VAL QG2 21240.0 e
HN 12 GLN HN 8762.0 e
HN 13 LYS+ HN 790.0 e
HN 97 TYR HD1 1381.0 e
HN 97 TYR HE1 971.0 e
HA 11 VAL HB 42730.0 e
HA 11 VAL QG1 83000.0 e
HA 11 VAL QG2 50040.0 e
HA 12 GLN HN 7481.0 e
HA 12 GLN HB2 1072.0 e
HB 11 VAL QG1 153000.0 e
HB 11 VAL QG2 121700.0 e
HB 12 GLN HN 12670.0 e
QG1 12 GLN HN 7171.0 e
QG1 97 TYR HE1 1657.0 e
QG2 12 GLN HN 9513.0 e
QG2 12 GLN HA 13220.0 e
QG2 15 ALA HA 3177.0 e
QG2 97 TYR HE1 1614.0 e

12 GLN
HN 12 GLN HA 17000.0 e
HN 12 GLN HB2 15900.0 e
HN 12 GLN HB3 2278.0 e
HN 12 GLN HG2 11250.0 e
HN 12 GLN HG3 7138.0 e
HN 13 LYS+ HN 15950.0 e
HN 13 LYS+ HA 224.0 e
HN 14 CYSS HN 1722.0 e
HA 12 GLN HB2 21090.0 e
HA 12 GLN HB3 19680.0 e
HA 12 GLN HG2 10550.0 e
HA 12 GLN HG3 10970.0 e
HA 13 LYS+ HN 3701.0 e
HB2 12 GLN HG3 152600.0 e
HB2 13 LYS+ HN 10610.0 e
HB2 13 LYS+ QG 5630.0*2e
HB3 13 LYS+ HN 7359.0 e
HG2 12 GLN HE22 5579.0 e
HG2 13 LYS+ HN 422.0 e
HG3 12 GLN HE22 4721.0 e
HG3 13 LYS+ HN 935.0 e

13 LYS+
HN 13 LYS+ HA 7797.0 e
HN 13 LYS+ QB 9660.0*2e
HN 13 LYS+ QG 4037.0*2e

HN 13 LYS+ QE 100.5*2e
HN 14 CYSS HN 18060.0 e
HN 15 ALA HA 184.0 e
HN 18 HEM HT2A 446.0 e
HN 18 HEM QT2 1025.0 e
HA 13 LYS+ QB 5900.0*2e
HA 13 LYS+ QG 5575.0*2e
HA 13 LYS+ QE 194.5*2e
QB 13 LYS+ QG 21222.5*4e
QB 14 CYSS HN 1581.5*2e
QB 18 HEM HT2A 886.5*2e
QB 18 HEM QT2 9305.0*2e
QB 82 PHE CZ 2366.0*4e
QB 82 PHE HZ 3807.5*2e
QG 14 CYSS HN 17.0*2e
QG 18 HEM QT2 8250.0*2e
QG 82 PHE CZ 2692.5*4e
QE 18 HEM QT2 84.0*2e
QE 82 PHE HZ 1192.0*2e
QE 85 ILE QD1 2751.5*2e
QE 94 LEU HB3 278.0*2e

14 CYSS
HN 14 CYSS HA 1011.0 e
HN 15 ALA HA 1923.0 e
HN 16 GLN HN 1268.0 e
HN 18 HEM HT2A 484.0 e
HN 18 HEM QT2 708.0 e
HA 15 ALA HA 1503.0 e

15 ALA
HN 15 ALA HA 20310.0 e
HN 15 ALA QB 39820.0 e
HN 16 GLN HN 6743.0 e
HN 17 CYSS HN 1033.0 e
HN 18 HEM HN 612.0 e
HA 15 ALA QB 98960.0 e
HA 16 GLN HN 3974.0 e
HA 16 GLN HE21 274.0 e
HA 18 HEM HN 22480.0 e
HA 18 HEM HB2 3585.0 e
HA 18 HEM HB3 1372.5 e
QB 16 GLN HN 12840.0 e
QB 17 CYSS HN 2330.0 e
QB 18 HEM HN 5297.0 e

16 GLN
HN 16 GLN HB2 17930.0 e
HN 16 GLN HB3 16630.0 e
HN 16 GLN HG2 4879.0 e
HN 16 GLN HG3 8614.0 e
HN 16 GLN HE21 385.0 e
HN 16 GLN HE22 85.0 e
HN 17 CYSS HN 16080.0 e
HN 18 HEM HN 1598.0 e
HB2 16 GLN HG2 18370.0 e
HB2 16 GLN HE21 321.0 e
HB2 17 CYSS HN 4373.0 e
HB2 18 HEM HN 281.0 e
HB3 16 GLN HG2 6822.0 e
HB3 16 GLN HG3 15620.0 e
HB3 16 GLN HE21 178.0 e
HB3 16 GLN HE22 200.0 e
HB3 17 CYSS HN 6383.0 e
HB3 17 CYSS HA 1128.0 e
HB3 18 HEM HN 621.0 e
HG2 16 GLN HE21 3315.0 e
HG2 17 CYSS HN 2587.0 e
HG3 16 GLN HE21 4368.0 e
HG3 16 GLN HE22 1016.0 e
HG3 17 CYSS HN 2861.0 e
HG3 18 HEM HN 350.0 e
HE21 18 HEM HN 110.0 e

17 CYSS
HN 17 CYSS HA 15350.0 e
HN 17 CYSS HB3 1568.0 e
HN 18 HEM HN 22180.0 e
HA 18 HEM HN 15090.0 e
HA 18 HEM HA 426.0 e
HA 28 THR HN 144.0 e
HA 28 THR HB 15460.0 e
HA 28 THR QG2 4515.0 e
HA 29 GLY HN 3660.0 e
HA 29 GLY HA1 323.0 e
HB3 18 HEM HBM 12680.0 e
HB3 18 HEM QM5 6482.0 e
HB3 27 LYS+ HN 1258.0 e
HB3 28 THR QG2 17950.0 e

18 HEM
HN 18 HEM HA 7844.0 e
HN 18 HEM HB2 5701.0 e
HN 18 HEM HB3 4394.0 e
HN 19 THR HN 2628.0 e
HN 19 THR HA 361.0 e
HN 28 THR HB 394.0 e
HN 29 GLY HN 137.0 e
HA 18 HEM HB3 35380.0 e
HA 19 THR HN 36430.0 e
HA 19 THR HA 2082.0 e
HA 19 THR HB 604.0 e
HA 19 THR QG2 727.5 e
HA 31 ASN HN 170.0 e
HA 31 ASN HA 859.0 e
HB3 19 THR HN 7015.0 e
HB3 19 THR HA 1372.0 e
HB3 19 THR HB 443.0 e
HB3 32 LEU HN 436.5 e
HB3 32 LEU HA 775.5 e
HB3 32 LEU QD1 10450.0 e
HB3 32 LEU QD2 2965.0 e
HD1 19 THR HN 1514.0 e
HD1 31 ASN HA 871.0 e
HD1 32 LEU QD2 274.0 e
HAP71 18 HEM HAP72 71750.0 e
HAP71 18 HEM HBP73 5808.0 e
HAP71 18 HEM HBP74 15695.0 e
HAP71 18 HEM QM8 3220.0 e
HAP71 18 HEM HGM 9430.0 e
HAP71 18 HEM HAP61 999.5 e
HAP71 18 HEM HAP62 3879.0 e
HAP71 18 HEM HBP64 1140.5 e
HAP71 32 LEU QD1 949.0 e
HAP71 35 LEU QD1 961.0 e
HAP71 40 THR HA 616.5 e
HAP71 40 THR HB 134.0 e
HAP71 40 THR QG2 732.0 e
HAP71 41 GLY HN 109.0 e

HAP71 59 TRP HD1 1398.0 e
HAP71 59 TRP HE1 2846.0 e
HAP71 59 TRP HZ2 8298.0 e
HAP71 59 TRP HH2 994.0 e
HAP72 18 HEM HBP73 16950.0 e
HAP72 18 HEM HBP74 18795.0 e
HAP72 18 HEM QM8 5830.0 e
HAP72 18 HEM HGM 26445.0 e
HAP72 18 HEM HAP61 212.0 e
HAP72 32 LEU QD1 1897.5 e
HAP72 32 LEU QD2 2212.5 e
HAP72 35 LEU QD1 3026.5 e
HAP72 35 LEU QD2 621.5 e
HAP72 40 THR HA 3803.5 e
HAP72 40 THR QG2 3071.0 e
HAP72 59 TRP HD1 2381.0 e
HAP72 59 TRP HE1 14855.0 e
HAP72 59 TRP HH2 3588.5 e
HAP72 64 LEU QD1 2023.5 e
HBP73 18 HEM QM8 5075.0 e
HBP73 59 TRP HE1 987.0 e
HBP74 18 HEM QM8 1316.0 e
HBP74 18 HEM HAP61 65.0 e
HBP74 35 LEU QD1 2019.0 e
HBP74 59 TRP HE1 3066.0 e
QM8 18 HEM QM1 1579.0 e
QM8 35 LEU QD1 4757.0 e
QM8 35 LEU QD2 4107.0 e
QM8 59 TRP HE1 851.5 e
QM8 59 TRP HZ2 970.0 e
QM8 64 LEU QD1 3627.0 e
QM8 67 TYR HB3 3350.0 e
QM1 18 HEM HT2A 1850.0 e
QM1 18 HEM QT2 45530.0 e
QM1 64 LEU QD1 4211.0 e
QM1 68 LEU QD1 10820.0 e
QM1 68 LEU QD2 41710.0 e
QM1 82 PHE CZ 585.0*2e
QM1 85 ILE QD1 5833.0 e
QM1 94 LEU QD1 30400.0 e
QM1 94 LEU QD2 36850.0 e
QM1 98 LEU QD1 33210.0 e
QM1 98 LEU QD2 3655.0 e
HT2A 18 HEM QT2 35680.0 e
HT2A 18 HEM HAM 10010.0 e
HT2A 18 HEM QM3 2920.0 e
HT2A 68 LEU QD2 196.0 e
HT2A 82 PHE CG 446.5*2e
HT2A 82 PHE CZ 992.5*2e
HT2A 82 PHE HZ 1055.0 e
HT2A 85 ILE QD1 717.0 e
HT2A 94 LEU QD2 282.0 e
QT2 18 HEM HAM 4945.0 e
QT2 68 LEU HN 1126.0 e
QT2 68 LEU HA 1316.0 e
QT2 68 LEU HB3 916.0 e
QT2 68 LEU QD1 9096.0 e
QT2 68 LEU QD2 46710.0 e
QT2 82 PHE CG 2824.0*2e
QT2 82 PHE CZ 16050.0*2e
QT2 82 PHE HZ 7256.0 e
QT2 85 ILE HN 639.0 e
QT2 85 ILE HA 1638.0 e
QT2 85 ILE HG12 12990.0 e
QT2 85 ILE HG13 14040.0 e
QT2 85 ILE QD1 54520.0 e
QT2 94 LEU HN 467.0 e
QT2 94 LEU HB3 2242.0 e
QT2 94 LEU QD1 11070.0 e
QT2 94 LEU QD2 60690.0 e
QT2 98 LEU QD1 3412.0 e
HAM 18 HEM QM3 5770.0 e
QM3 18 HEM HT4A 842.0 e
QM3 18 HEM QT4 14825.0 e
QM3 82 PHE CG 1708.5*2e
HT4A 18 HEM QT4 26860.0 e
HT4A 18 HEM HBM 2903.0 e
HT4A 28 THR QG2 6992.0 e
QT4 18 HEM HBM 4244.0 e
QT4 18 HEM QM5 1801.0 e
QT4 28 THR QG2 18380.0 e
QT4 81 ILE HN 2640.0 e
QT4 81 ILE QG2 2751.0 e
QT4 81 ILE HG12 3248.0 e
QT4 81 ILE QD1 1097.0 e
HBM 18 HEM QM5 21220.0 e
HBM 28 THR HB 2384.0 e
HBM 28 THR QG2 6353.0 e
HBM 80 MET HA 297.0 e
QM5 18 HEM HAP61 24925.0 e
QM5 18 HEM HAP62 13940.0 e
QM5 18 HEM HBP63 14790.0 e
QM5 18 HEM HBP64 2475.0 e
QM5 28 THR HA 6128.0 e
QM5 28 THR QG2 46150.0 e
QM5 29 GLY HN 870.0 e
QM5 29 GLY HA1 15360.0 e
QM5 29 GLY HA2 3904.0 e
QM5 30 PRO HD2 1438.5 e
QM5 30 PRO HD3 3740.0 e
QM5 46 PHE HD2 120.0 e
QM5 46 PHE HE1 181.0 e
QM5 46 PHE HZ 240.0 e
QM5 48 TYR HB3 2693.0 e
QM5 49 THR QG2 3108.0 e
QM5 79 LYS+ HN 627.0 e
QM5 79 LYS+ HG2 7150.0 e
QM5 79 LYS+ HG3 15430.0 e
QM5 79 LYS+ QE 1353.0*2e
QM5 80 MET HN 2055.0 e
QM5 80 MET HA 7386.0 e
QM5 81 ILE QD1 164.0 e
HAP61 18 HEM HAP62 26000.0 e
HAP61 18 HEM HBP63 6125.0 e
HAP61 18 HEM HBP64 4067.0 e
HAP61 29 GLY HA1 2975.5 e
HAP61 30 PRO HG2 1192.0 e
HAP61 30 PRO HD2 1791.5 e
HAP61 30 PRO HD3 1151.0 e
HAP61 46 PHE HE1 150.0 e
HAP61 46 PHE HE2 11800.0 e
HAP61 46 PHE HZ 7150.0 e
HAP61 79 LYS+ HN 322.0 e
HAP61 79 LYS+ QE 248.5*2e

HAP62 18 HEM HBP63 34180.0 e
HAP62 30 PRO HD3 3960.5 e
HBP63 18 HEM HBP64 10230.0 e
HBP63 78 THR HG1 846.0 e
HBP63 79 LYS+ HN 656.0 e
HBP63 80 MET HN 1460.0 e
HBP64 30 PRO HD3 707.0 e
HBP64 78 THR HG1 1212.0 e

19 THR
HN 19 THR HA 6561.0 e
HN 19 THR HB 1682.0 e
HN 19 THR QG2 15700.0 e
HN 19 THR HG1 8581.0 e
HN 20 VAL HN 862.0 e
HN 31 ASN HN 468.0 e
HN 31 ASN HA 10420.0 e
HN 31 ASN HB2 510.0 e
HN 31 ASN HB3 1694.0 e
HN 32 LEU HN 2432.0 e
HA 19 THR HB 19270.0 e
HA 19 THR QG2 41110.0 e
HA 19 THR HG1 2817.0 e
HA 20 VAL HN 19870.0 e
HA 20 VAL QG1 8091.0 e
HA 20 VAL QG2 8136.0 e
HA 21 GLU- HN 583.0 e
HA 31 ASN HA 944.0 e
HA 31 ASN HB2 199.0 e
HA 31 ASN HB3 638.0 e
HB 19 THR QG2 47620.0 e
HB 19 THR HG1 2989.0 e
HB 20 VAL HN 11120.0 e
HB 20 VAL QG1 1844.0 e
HB 20 VAL QG2 2471.0 e
HB 21 GLU- HN 861.0 e
HB 24 GLY HN 146.0 e
HB 24 GLY HA2 609.0 e
HB 31 ASN HA 487.0 e
HB 31 ASN HB2 265.0 e
HB 31 ASN HB3 2314.0 e
HB 32 LEU HN 291.0 e
QG2 19 THR HG1 2969.0 e
QG2 20 VAL HN 1463.0 e
QG2 22 LYS+ HN 12330.0 e
HG1 21 GLU- HN 501.0 e
HG1 22 LYS+ HA 271.0 e
HG1 24 GLY HN 224.0 e
HG1 24 GLY HA2 994.0 e
HG1 31 ASN HN 900.0 e
HG1 31 ASN HA 6267.0 e
HG1 31 ASN HB2 6315.0 e
HG1 31 ASN HB3 5099.0 e

20 VAL
HN 20 VAL HA 1278.0 e
HN 20 VAL HB 11540.0 e
HN 20 VAL QG1 8387.0 e
HN 20 VAL QG2 28360.0 e
HN 21 GLU- HN 2571.0 e
HN 31 ASN HB3 341.0 e
HA 20 VAL HB 7996.0 e
HA 20 VAL QG1 9160.0 e
HA 20 VAL QG2 3819.0 e
HB 20 VAL QG1 38910.0 e
HB 20 VAL QG2 55920.0 e
HB 97 TYR HD1 1303.0 e
HB 97 TYR HE1 2029.0 e
HB 101 ALA QB 4321.0 e
QG1 21 GLU- HN 884.0 e
QG1 97 TYR HE1 7148.0 e
QG1 98 LEU QD2 6258.0 e
QG2 21 GLU- HN 1880.0 e
QG2 33 HIS QB 1252.5*2e
QG2 97 TYR HE1 2680.0 e
QG2 101 ALA HA 3952.0 e

21 GLU-
HN 21 GLU- HA 492.0 e
HN 21 GLU- QB 729.0*2e
HN 22 LYS+ HN 391.0 e
HA 21 GLU- QB 476.0*2e
HA 22 LYS+ HN 2972.0 e
QB 22 LYS+ HN 793.0*2e

22 LYS+
HN 22 LYS+ HA 7443.0 e
HN 22 LYS+ HB2 17550.0 e
HN 22 LYS+ HB3 2267.0 e
HN 22 LYS+ QG 7345.0*2e
HN 22 LYS+ QD 859.0*2e
HN 22 LYS+ QE 690.5*2e
HN 23 GLY HN 396.0 e
HA 22 LYS+ HB2 9562.0 e
HA 22 LYS+ HB3 19290.0 e
HA 22 LYS+ QG 9315.0*2e
HA 22 LYS+ QD 6535.0*2e
HA 22 LYS+ QE 4577.5*2e
HA 23 GLY HN 17150.0 e
HA 23 GLY HA1 1280.0 e
HA 23 GLY HA2 276.0 e
HA 24 GLY HN 695.0 e
HB2 22 LYS+ QG 33905.0*2e
HB2 23 GLY HN 1196.0 e
HB3 22 LYS+ QE 5060.0*2e
HB3 23 GLY HN 3684.0 e
QG 22 LYS+ QE 356.5*4e
QG 23 GLY HN 771.5*2e
QD 22 LYS+ QE 4272.5*4e
QD 23 GLY HN 1111.5*2e
QE 23 GLY HN 147.0*2e

23 GLY
HN 23 GLY HA1 3951.0 e
HN 23 GLY HA2 1593.0 e
HN 24 GLY HN 2450.0 e
HA1 24 GLY HN 489.0 e

24 GLY
HN 24 GLY HA2 2409.0 e
HN 25 LYS+ HN 653.0 e
HA1 25 LYS+ HN 309.0 e
HA2 25 LYS+ HN 1482.0 e

25 LYS+
HN 25 LYS+ HA 13870.0 e
HN 25 LYS+ HB2 8207.0 e
HN 25 LYS+ HB3 10530.0 e
HN 25 LYS+ HG2 8051.0 e
HN 25 LYS+ HG3 8404.0 e
HN 25 LYS+ QD 4191.5*2e

HN 25 LYS+ QE 921.5*2e
HA 25 LYS+ HB2 17340.0 e
HA 25 LYS+ HB3 9470.0 e
HA 25 LYS+ HG2 7696.0 e
HA 25 LYS+ HG3 9896.0 e
HA 25 LYS+ QD 7880.0*2e
HA 25 LYS+ QE 500.0*2e
HA 26 HIS HD2 461.0 e
HB2 25 LYS+ QE 8355.0*2e
HB2 26 HIS HN 7861.0 e
HB3 25 LYS+ QE 561.5*2e
HB3 26 HIS HN 6457.0 e
HG2 26 HIS HN 3528.0 e
HG3 25 LYS+ QE 1560.0*2e
HG3 26 HIS HN 2768.0 e

26 HIS

HN 26 HIS HB2 6546.0 e
HN 26 HIS HB3 4715.0 e
HN 26 HIS HD2 952.0 e
HN 27 LYS+ HA 423.0 e
HN 31 ASN HN 197.0 e
HA 26 HIS HB2 270.0 e
HA 26 HIS HB3 494.0 e
HA 31 ASN HN 811.0 e
HB2 27 LYS+ HN 458.0 e
HB3 27 LYS+ HN 1293.0 e
HB3 31 ASN HN 293.0 e
HD2 30 PRO HB2 110.0 e
HE1 30 PRO HA 3588.0 e
HE1 30 PRO HB2 6600.0 e
HE1 30 PRO HB3 34880.0 e
HE1 30 PRO HG2 1026.0 e
HE1 30 PRO HG3 6554.0 e
HE1 30 PRO HD3 298.0 e
HE1 31 ASN HN 11040.0 e
HE1 31 ASN HA 1212.0 e
HE1 31 ASN HB2 6101.0 e
HE1 31 ASN HB3 15715.0 e
HE1 44 PRO HA 158.0 e
HE1 46 PHE HB2 2430.0 e
HE1 46 PHE HD1 289.0 e
HE1 46 PHE HD2 757.0 e

27 LYS+

HN 27 LYS+ HA 253.0 e
HN 27 LYS+ QB 11330.0*2e
HA 27 LYS+ QB 1696.5*2e

28 THR

HN 28 THR HA 2080.0 e
HN 28 THR QG2 304.0 e
HN 29 GLY HN 40.0 e
HA 29 GLY HN 18620.0 e
HA 29 GLY HA1 962.0 e
HB 28 THR QG2 139500.0 e
HB 29 GLY HA2 1389.5 e
QG2 29 GLY HN 5253.0 e
QG2 79 LYS+ HG2 485.0 e
QG2 79 LYS+ QE 142.0*2e
QG2 81 ILE HN 440.0 e

29 GLY

HN 29 GLY HA1 4213.0 e
HN 29 GLY HA2 7645.0 e
HN 30 PRO HA 901.0 e
HN 30 PRO HB3 365.0 e
HN 30 PRO HG2 1079.0 e
HN 30 PRO HG3 529.0 e
HN 30 PRO HD2 504.0 e
HN 30 PRO HD3 752.0 e
HN 31 ASN HN 393.0 e
HA1 31 ASN HN 283.0 e
HA1 46 PHE HE2 3416.5 e
HA1 46 PHE HZ 12600.0 e
HA2 30 PRO HA 897.0 e
HA2 30 PRO HG3 384.0 e
HA2 30 PRO HD2 2794.0 e
HA2 30 PRO HD3 4886.5 e
HA2 46 PHE HE1 1307.5 e
HA2 46 PHE HZ 2901.5 e

30 PRO

HA 30 PRO HB2 17280.0 e
HA 30 PRO HG2 5779.0 e
HA 30 PRO HG3 27570.0 e
HA 30 PRO HD2 2954.0 e
HA 30 PRO HD3 3873.0 e
HA 31 ASN HN 23040.0 e
HA 43 ALA QB 2705.0 e
HB2 30 PRO HG2 17630.0 e
HB2 30 PRO HG3 116900.0 e
HB2 30 PRO HD2 2956.5 e
HB2 30 PRO HD3 6568.0 e
HB2 31 ASN HN 6643.0 e
HB2 46 PHE HD1 373.0 e
HB3 30 PRO HG2 5575.0 e
HB3 30 PRO HD2 3376.0 e
HB3 30 PRO HD3 1674.0 e
HB3 31 ASN HN 2659.0 e
HG2 30 PRO HD2 15270.0 e
HG2 30 PRO HD3 20160.0 e
HG2 46 PHE HD1 719.0 e
HG2 46 PHE HD2 464.0 e
HG2 46 PHE HE1 236.0 e
HG3 30 PRO HD2 12435.0 e
HG3 30 PRO HD3 17950.0 e
HG3 31 ASN HN 2584.0 e
HG3 43 ALA QB 5809.0 e
HG3 46 PHE HD1 1499.0 e
HG3 46 PHE HE1 111.0 e
HD2 46 PHE HE1 1217.5 e
HD2 46 PHE HE2 933.0 e
HD2 46 PHE HZ 2103.5 e
HD3 31 ASN HN 187.0 e
HD3 46 PHE HD1 819.0 e
HD3 46 PHE HE1 105.0 e
HD3 46 PHE HE2 2702.0 e
HD3 46 PHE HZ 5530.0 e

31 ASN

HN 31 ASN HA 6352.0 e
HN 31 ASN HB2 11900.0 e
HN 31 ASN HB3 15580.0 e
HN 32 LEU HN 655.0 e
HN 32 LEU QD2 607.0 e
HN 46 PHE HB2 493.0 e
HN 46 PHE HD1 270.0 e
HA 31 ASN HB2 10390.0 e
HA 31 ASN HB3 10600.0 e

HA 32 LEU HN 24430.0 e
HB2 32 LEU HN 701.0 e
32 LEU
HN 32 LEU HA 1053.0 e
HN 32 LEU QB 697.0*2e
HN 32 LEU HG 10900.0 e
HN 32 LEU QD1 915.0 e
HN 32 LEU QD2 1359.0 e
HN 33 HIS HN 1618.0 e
HA 32 LEU QB 1367.5*2e
HA 32 LEU HG 4468.0 e
HA 32 LEU QD1 316.0 e
HA 35 LEU QD1 787.0 e
HA 35 LEU QD2 699.0 e
QB 35 LEU QD2 9580.0*2e
QD1 64 LEU QD1 2225.0 e
QD1 98 LEU QD1 184.0 e
QD2 35 LEU QD1 13490.0 e
QD2 35 LEU QD2 1138.0 e
33 HIS
HN 33 HIS HA 321.0 e
HN 33 HIS QB 249.5*2e
HN 34 GLY HA2 234.0 e
34 GLY
HN 34 GLY HA1 2322.0 e
HN 34 GLY HA2 1878.0 e
HN 35 LEU HN 3559.0 e
HA1 35 LEU HN 200.0 e
HA2 35 LEU HN 1704.0 e
HA2 102 THR QG2 1524.0 e
35 LEU
HN 35 LEU HA 8892.0 e
HN 35 LEU HB2 31490.0 e
HN 35 LEU HB3 13850.0 e
HN 35 LEU QD1 11190.0 e
HN 35 LEU QD2 4831.0 e
HN 36 PHE HN 4522.0 e
HA 35 LEU HB2 7843.0 e
HA 35 LEU HB3 41680.0 e
HA 35 LEU HG 5936.0 e
HA 35 LEU QD1 53390.0 e
HA 35 LEU QD2 20800.0 e
HA 36 PHE HN 1560.0 e
HB2 35 LEU QD1 7144.0 e
HB2 35 LEU QD2 13690.0 e
HB2 36 PHE CG 6645.0*2e
HB2 36 PHE CZ 2772.0*2e
HB2 36 PHE HZ 2973.0 e
HB3 35 LEU QD1 23560.0 e
HB3 35 LEU QD2 25710.0 e
HB3 36 PHE HN 621.0 e
HB3 36 PHE CG 2766.5*2e
HB3 36 PHE CZ 3694.5*2e
HB3 36 PHE HZ 859.0 e
HG 35 LEU QD1 18960.0 e
HG 35 LEU QD2 24350.0 e
HG 36 PHE HN 812.0 e
HG 36 PHE HA 3073.0 e
HG 59 TRP HD1 3750.0 e
HG 64 LEU QD1 537.0 e
HG 64 LEU QD2 2633.0 e
QD1 36 PHE HN 2255.0 e
QD1 36 PHE CG 1506.5*2e
QD1 40 THR HA 1265.0 e
QD1 59 TRP HD1 24960.0 e
QD1 59 TRP HE3 776.0 e
QD1 59 TRP HE1 5601.0 e
QD1 64 LEU QD2 5534.0 e
QD2 36 PHE HN 3316.0 e
QD2 36 PHE HA 1855.0 e
QD2 36 PHE CG 10360.0*2e
QD2 59 TRP HN 561.0 e
QD2 59 TRP HD1 4203.0 e
QD2 59 TRP HE3 2085.0 e
QD2 59 TRP HE1 633.0 e
QD2 59 TRP HZ2 389.0 e
QD2 64 LEU QD1 15380.0 e
QD2 64 LEU QD2 16410.0 e
QD2 98 LEU QD1 9681.0 e
QD2 102 THR HN 644.0 e
QD2 102 THR HG1 1078.0 e
36 PHE
HN 36 PHE HA 7567.0 e
HN 36 PHE HB2 11380.0 e
HN 36 PHE HB3 8967.0 e
HN 36 PHE CG 12640.0*2e
HN 36 PHE CZ 1891.5*2e
HN 37 GLY HN 878.0 e
HA 36 PHE HB2 10100.0 e
HA 36 PHE HB3 13070.0 e
HA 36 PHE CG 6190.0*2e
HA 36 PHE CZ 958.0*2e
HA 37 GLY HN 20460.0 e
HB2 36 PHE CG 14905.0*2e
HB2 36 PHE CZ 1902.5*2e
HB2 37 GLY HN 2252.0 e
HB2 99 LYS+ HA 1913.0 e
HB2 102 THR HG1 1122.0 e
HB3 36 PHE CG 16630.0*2e
HB3 36 PHE CZ 961.0*2e
HB3 37 GLY HN 3444.0 e
HB3 102 THR HG1 486.0 e
CG 36 PHE CZ 25200.0*4e
CG 36 PHE HZ 6630.0*2e
CG 37 GLY HN 1302.5*2e
CG 59 TRP HN 106.5*2e
CG 60 LYS+ HA 7380.0*2e
CG 60 LYS+ QB 571.8*4e
CG 60 LYS+ QG 498.5*4e
CG 61 GLU- HN 1496.5*2e
CG 61 GLU- HA 2377.0*2e
CG 64 LEU QD1 353.5*2e
CG 64 LEU QD2 3673.5*2e
CG 98 LEU HA 314.0*2e
CG 98 LEU HB2 704.0*2e
CG 98 LEU QD1 755.0*2e
CG 99 LYS+ HN 248.5*2e
CG 99 LYS+ HA 5065.0*2e
CG 99 LYS+ QB 2840.0*4e
CG 99 LYS+ QG 342.2*4e
CG 102 THR QG2 657.5*2e
CG 102 THR HG1 1162.0*2e
CZ 36 PHE HZ 39000.0*2e
CZ 37 GLY HN 97.0*2e

CZ	60 LYS+ HA	970.0*2e
CZ	61 GLU- HN	2533.0*2e
CZ	61 GLU- HA	4640.0*2e
CZ	61 GLU- QB	328.5*4e
CZ	62 GLU- HN	157.5*2e
CZ	64 LEU QD1	1924.0*2e
CZ	64 LEU QD2	11455.0*2e
CZ	95 ILE HA	1132.0*2e
CZ	95 ILE HB	810.5*2e
CZ	95 ILE QG2	1734.0*2e
CZ	95 ILE QD1	268.0*2e
CZ	98 LEU HN	958.0*2e
CZ	98 LEU HA	1481.0*2e
CZ	98 LEU HB2	4797.5*2e
CZ	98 LEU HB3	10135.0*2e
CZ	98 LEU QD1	5505.0*2e
CZ	98 LEU QD2	4560.5*2e
CZ	99 LYS+ HN	2677.5*2e
CZ	99 LYS+ HA	8805.0*2e
CZ	99 LYS+ QG	550.0*4e
CZ	99 LYS+ QD	5220.0*4e
CZ	102 THR QG2	810.0*2e
HZ	60 LYS+ HA	587.0 e
HZ	61 GLU- HN	516.0 e
HZ	61 GLU- HA	3345.0 e
HZ	64 LEU QD1	2823.0 e
HZ	64 LEU QD2	19000.0 e
HZ	95 ILE HA	4809.0 e
HZ	95 ILE HB	2174.0 e
HZ	95 ILE QG2	4124.0 e
HZ	95 ILE HG13	27370.0 e
HZ	95 ILE QD1	842.0 e
HZ	98 LEU HA	952.0 e
HZ	98 LEU HB2	3680.0 e
HZ	98 LEU HB3	5985.0 e
HZ	98 LEU QD1	5590.0 e
HZ	98 LEU QD2	1830.0 e
HZ	99 LYS+ HA	7500.0 e
HZ	99 LYS+ QB	1591.0*2e
HZ	99 LYS+ QG	375.0*2e
HZ	99 LYS+ QD	2797.0*2e
37 GLY		
HN	37 GLY HA1	1938.0 e
HN	37 GLY HA2	6906.0 e
HN	38 ARG+ HN	7150.0 e
HN	58 THR QG2	5224.0 e
HN	60 LYS+ HA	388.0 e
HA1	58 THR QG2	4052.0 e
38 ARG+		
HN	38 ARG+ HA	1552.0 e
HN	38 ARG+ HB2	12510.0 e
HN	38 ARG+ HB3	7031.0 e
HN	38 ARG+ QG	718.0*2e
HA	38 ARG+ HB2	512.0 e
HA	38 ARG+ HB3	2641.0 e
HB2	59 TRP HD1	2334.0 e
HB3	38 ARG+ QD	26040.0*2e
HB3	40 THR HN	225.0 e
HB3	59 TRP HD1	1775.0 e
QG	38 ARG+ QD	1153.0*4e
39 LYS+		
HN	58 THR HA	181.0 e
HN	59 TRP HN	1145.0 e
HB2	40 THR HN	5738.0 e
HB3	40 THR HN	5187.0 e
QG	40 THR HN	452.0*2e
40 THR		
HN	40 THR HA	6117.0 e
HN	40 THR HB	2917.0 e
HN	40 THR QG2	34180.0 e
HN	40 THR HG1	989.0 e
HN	41 GLY HN	734.0 e
HN	56 GLY HN	253.0 e
HN	57 ILE HN	1427.0 e
HN	57 ILE HG13	400.0 e
HN	57 ILE QD1	4411.0 e
HN	59 TRP HB3	127.0 e
HA	40 THR HB	2720.0 e
HA	40 THR QG2	17210.0 e
HA	40 THR HG1	147.0 e
HA	41 GLY HN	7328.0 e
HA	59 TRP HD1	4970.0 e
HA	59 TRP HE3	633.0 e
HA	59 TRP HE1	16510.0 e
HB	40 THR QG2	15430.0 e
HB	40 THR HG1	2666.0 e
HB	41 GLY HN	1269.0 e
HB	56 GLY HN	1332.0 e
HB	59 TRP HE1	473.0 e
QG2	40 THR HG1	722.0 e
QG2	41 GLY HN	2621.0 e
QG2	41 GLY HA2	4592.0 e
QG2	55 LYS+ HN	2171.0 e
QG2	55 LYS+ HB3	6355.0 e
QG2	55 LYS+ QD	222.0*2e
QG2	56 GLY HN	6879.0 e
QG2	59 TRP HN	823.0 e
QG2	59 TRP HD1	1901.0 e
QG2	59 TRP HE3	3837.0 e
QG2	59 TRP HE1	11780.0 e
QG2	59 TRP HZ3	1883.0 e
QG2	59 TRP HH2	3348.0 e
QG2	74 TYR CG	687.0*2e
HG1	41 GLY HN	829.0 e
HG1	41 GLY HA2	237.0 e
HG1	56 GLY HN	9919.0 e
HG1	57 ILE HN	1260.0 e
HG1	59 TRP HE1	519.0 e
41 GLY		
HN	41 GLY HA1	7759.0 e
HN	41 GLY HA2	6419.0 e
HN	42 GLN HN	2079.0 e
HN	53 LYS+ HA	548.0 e
HN	56 GLY HN	313.0 e
HN	59 TRP HD1	504.0 e
HN	59 TRP HE1	2909.0 e
HA1	42 GLN HN	5414.0 e
HA1	55 LYS+ HN	1004.0 e
HA2	42 GLN HN	9838.0 e
HA2	42 GLN HG2	10780.0 e
HA2	42 GLN HG3	3559.0 e
HA2	53 LYS+ HA	17150.0 e
42 GLN		
HN	42 GLN HA	4036.0 e

HN	42 GLN	HB2	3520.0 e
HN	42 GLN	HB3	2491.0 e
HN	42 GLN	HG2	4273.0 e
HN	42 GLN	HG3	14740.0 e
HN	43 ALA	HN	5763.0 e
HA	42 GLN	HB2	13900.0 e
HA	42 GLN	HB3	2642.0 e
HA	42 GLN	HG2	3674.0 e
HA	42 GLN	HG3	6855.0 e
HA	42 GLN	HE22	227.0 e
HA	43 ALA	HN	2478.0 e
HA	43 ALA	QB	139.0 e
HB2	42 GLN	HE22	108.0 e
HG2	42 GLN	HE22	2529.0 e
HG3	42 GLN	HE22	11370.0 e
HE22	53 LYS+	HA	103.0 e
43 ALA			
HN	43 ALA	QB	38160.0 e
HA	43 ALA	QB	3868.0 e
QB	46 PHE	HN	2866.0 e
QB	46 PHE	HB2	2078.0 e
QB	46 PHE	HD1	374.0 e
QB	47 THR	HN	2790.0 e
44 PRO			
HA	44 PRO	HB2	8526.0 e
HA	44 PRO	HB3	10950.0 e
HA	44 PRO	HG2	1692.0 e
HA	44 PRO	HG3	2460.0 e
HA	44 PRO	HD2	639.0 e
HB2	45 GLY	HN	847.0 e
HB3	45 GLY	HN	585.0 e
45 GLY			
HN	45 GLY	HA1	493.0 e
HN	45 GLY	HA2	1395.0 e
HN	46 PHE	HN	920.0 e
HA1	46 PHE	HN	3776.0 e
HA2	46 PHE	HN	557.0 e
46 PHE			
HN	46 PHE	HA	7691.0 e
HN	46 PHE	HB2	14450.0 e
HN	46 PHE	HB3	12380.0 e
HN	47 THR	HA	762.0 e
HA	46 PHE	HB2	22150.0 e
HA	46 PHE	HB3	3164.0 e
HA	47 THR	HN	9220.0 e
HB2	46 PHE	HD1	5083.0 e
HB2	47 THR	HN	635.0 e
HB2	48 TYR	CG	879.5*2e
HB3	46 PHE	HD1	3290.0 e
HD1	46 PHE	HE1	139.0 e
HD1	46 PHE	HZ	6560.0 e
HD1	47 THR	HA	1038.0 e
HD1	48 TYR	HA	215.0 e
HD2	46 PHE	HE1	89.0 e
HD2	48 TYR	HN	734.0 e
HD2	48 TYR	CG	1655.0*2e
HE1	46 PHE	HZ	17295.0 e
47 THR			
HN	47 THR	HA	3515.0 e
HN	47 THR	HB	7865.0 e
HN	47 THR	QG2	5712.0 e
HN	48 TYR	HN	1038.0 e
HA	47 THR	HB	9830.0 e
HA	47 THR	QG2	49380.0 e
HA	48 TYR	HN	27040.0 e
HB	47 THR	QG2	65140.0 e
HB	48 TYR	HN	1408.0 e
QG2	48 TYR	HN	7922.0 e
48 TYR			
HN	48 TYR	HA	7290.0 e
HN	48 TYR	HB2	4853.0 e
HN	48 TYR	HB3	2745.0 e
HN	49 THR	HN	719.0 e
HA	48 TYR	HB3	3325.0 e
HA	49 THR	HN	10970.0 e
HB2	49 THR	HN	2917.0 e
HB2	53 LYS+	HN	2162.0 e
HB3	49 THR	HN	1444.0 e
CG	52 ASN	HB3	5020.0*2e
CG	53 LYS+	HA	130.0*2e
49 THR			
HN	49 THR	HA	4216.0 e
HN	49 THR	QG2	14500.0 e
HN	50 ASP-	HN	411.0 e
HN	52 ASN	HN	828.0 e
HN	52 ASN	HB2	1880.0 e
HN	52 ASN	HB3	8474.0 e
HA	49 THR	QG2	47620.0 e
HA	50 ASP-	HN	14140.0 e
HB	50 ASP-	HN	5976.0 e
QG2	50 ASP-	HN	3692.0 e
QG2	52 ASN	HN	2382.0 e
QG2	78 THR	HN	414.0 e
QG2	78 THR	HA	7989.0 e
QG2	78 THR	HB	1162.0 e
QG2	79 LYS+	HN	7652.0 e
QG2	79 LYS+	QE	2472.0*2e
QG2	80 MET	HN	727.0 e
50 ASP-			
HN	50 ASP-	HA	24660.0 e
HN	50 ASP-	QB	9840.0*2e
HN	51 ALA	HN	6062.0 e
HA	50 ASP-	QB	17770.0*2e
HA	51 ALA	HN	750.0 e
HA	52 ASN	HN	923.0 e
HA	53 LYS+	HN	4965.0 e
HA	53 LYS+	HA	1756.0 e
HA	53 LYS+	QB	7255.0*2e
HA	53 LYS+	QG	2075.5*2e
HA	53 LYS+	QD	4118.5*2e
HA	53 LYS+	QE	3259.0*2e
HA	54 ASN	HN	1544.0 e
HA	54 ASN	HD21	885.0 e
QB	51 ALA	HN	6835.0*2e
QB	51 ALA	HA	1231.0*2e
QB	52 ASN	HN	85.5*2e
QB	54 ASN	HD21	2599.5*2e
QB	54 ASN	HD22	1767.0*2e
51 ALA			
HN	51 ALA	HA	7302.0 e
HN	51 ALA	QB	49030.0 e
HN	52 ASN	HN	5531.0 e
HA	51 ALA	QB	53480.0 e
HA	52 ASN	HN	1636.0 e

HA 54 ASN HN 4271.0 e
HA 54 ASN HB2 1169.0 e
HA 54 ASN HB3 170.0 e
HA 54 ASN HD21 355.0 e
HA 55 LYS+ HN 471.0 e
HA 75 ILE QG2 8638.0 e
QB 52 ASN HN 12480.0 e
QB 52 ASN HB2 6119.0 e
QB 78 THR HN 1719.0 e
QB 78 THR HA 2759.0 e
QB 78 THR HB 1949.0 e

52 ASN

HN 52 ASN HB2 11040.0 e
HN 52 ASN HB3 17740.0 e
HN 53 LYS+ HN 9033.0 e
HN 53 LYS+ QB 381.0*2e
HN 53 LYS+ QD 652.5*2e
HN 54 ASN HB2 365.0 e
HN 75 ILE QG2 2588.0 e
HB2 53 LYS+ HN 3943.0 e
HB3 53 LYS+ HN 3887.0 e

53 LYS+

HN 53 LYS+ HA 6819.0 e
HN 53 LYS+ QB 7880.0*2e
HN 53 LYS+ QG 6435.0*2e
HN 53 LYS+ QD 13490.0*2e
HN 53 LYS+ QE 143.0*2e
HN 54 ASN HN 7867.0 e
HN 55 LYS+ HN 466.0 e
HA 53 LYS+ QB 7865.0*2e
HA 53 LYS+ QG 13615.0*2e
HA 53 LYS+ QD 12265.0*2e
HA 53 LYS+ QE 2747.0*2e
QB 53 LYS+ QG 13610.0*4e
QB 54 ASN HN 2986.5*2e

54 ASN

HN 54 ASN HA 2421.0 e
HN 54 ASN HB2 10500.0 e
HN 54 ASN HB3 6415.0 e
HN 55 LYS+ HN 8933.0 e
HN 55 LYS+ HB3 2767.0 e
HB2 54 ASN HD21 11650.0 e
HB2 54 ASN HD22 5420.0 e
HB2 55 LYS+ HN 7219.0 e
HB2 55 LYS+ HA 271.0 e
HB3 54 ASN HD21 7338.0 e
HB3 55 LYS+ HN 7288.0 e

55 LYS+

HN 55 LYS+ HA 9179.0 e
HN 55 LYS+ HB2 2464.0 e
HN 55 LYS+ HB3 14290.0 e
HN 55 LYS+ QD 1722.0*2e
HN 55 LYS+ QE 886.5*2e
HN 56 GLY HN 2416.0 e
HN 56 GLY HA2 576.0 e
HN 57 ILE HG13 23.0 e
HA 55 LYS+ HB2 6032.0 e
HA 55 LYS+ HB3 9300.0 e
HA 55 LYS+ QG 1077.5*2e
HA 55 LYS+ QD 2723.0*2e
HA 56 GLY HN 583.0 e
HA 57 ILE HN 1438.0 e
HA 57 ILE QG2 1458.0 e
HB3 56 GLY HN 2757.0 e
HB3 57 ILE QD1 921.0 e
QG 74 TYR CZ 1874.0*4e
QE 74 TYR CG 443.0*4e

56 GLY

HN 56 GLY HA1 2668.0 e
HN 56 GLY HA2 7908.0 e
HN 57 ILE HN 4424.0 e
HN 57 ILE QD1 616.0 e
HA2 57 ILE HN 415.0 e
HA2 57 ILE HG12 4676.0 e

57 ILE

HN 57 ILE HA 2729.0 e
HN 57 ILE HB 3846.0 e
HN 57 ILE QG2 38040.0 e
HN 57 ILE HG12 15060.0 e
HN 57 ILE HG13 13490.0 e
HN 57 ILE QD1 6244.0 e
HN 58 THR HN 173.0 e
HA 57 ILE HB 6383.0 e
HA 57 ILE QG2 4032.0 e
HA 57 ILE HG12 766.0 e
HA 57 ILE HG13 1634.0 e
HA 57 ILE QD1 4622.0 e
HA 58 THR HN 10120.0 e
HB 57 ILE QG2 40380.0 e
HB 57 ILE HG12 37990.0 e
HB 58 THR HN 18810.0 e
HB 74 TYR CZ 1936.0*2e
QG2 57 ILE HG12 51640.0 e
QG2 57 ILE QD1 67760.0 e
QG2 58 THR HN 7789.0 e
QG2 74 TYR CZ 4426.5*2e
HG12 57 ILE QD1 25680.0 e
HG12 58 THR HN 1232.0 e
HG12 74 TYR CZ 7345.0*2e
HG13 57 ILE QD1 27480.0 e
HG13 58 THR HN 308.0 e
HG13 74 TYR CZ 3287.0*2e
QD1 58 THR HN 5638.0 e
QD1 58 THR HA 1517.0 e
QD1 58 THR QG2 1806.0 e
QD1 59 TRP HN 1081.0 e
QD1 59 TRP HB2 981.0 e
QD1 63 THR HA 106.0 e
QD1 63 THR HB 6901.0 e
QD1 63 THR QG2 17520.0 e
QD1 74 TYR CG 1610.5*2e
QD1 74 TYR CZ 13490.0*2e

58 THR

HN 58 THR HA 2211.0 e
HN 58 THR HB 15520.0 e
HN 58 THR QG2 3918.0 e
HN 63 THR QG2 3046.0 e
HA 58 THR HB 4947.0 e
HA 58 THR QG2 21010.0 e
HA 59 TRP HN 11580.0 e
HB 58 THR QG2 61080.0 e
HB 58 THR HG1 5821.0 e
QG2 58 THR HG1 3782.0 e
QG2 59 TRP HN 11260.0 e

	QG2	60 LYS+ HA	129.0 e
	QG2	60 LYS+ QB	901.0*2e
	HG1	60 LYS+ QB	790.5*2e
	HG1	60 LYS+ QG	2408.5*2e
	HG1	60 LYS+ QE	137.5*2e
59 TRP			
	HN	59 TRP HB2	5125.0 e
	HN	59 TRP HB3	4019.0 e
	HN	59 TRP HD1	4207.0 e
	HN	64 LEU QD1	302.0 e
	HB2	59 TRP HE3	1466.0 e
	HB2	59 TRP HZ3	286.0 e
	HB2	64 LEU QD1	2615.0 e
	HB2	64 LEU QD2	1453.0 e
	HB3	59 TRP HD1	9028.0 e
	HB3	59 TRP HE3	2107.0 e
	HD1	59 TRP HE1	22750.0 e
	HE3	59 TRP HE1	1013.0 e
	HE3	59 TRP HZ3	11920.0 e
	HE3	59 TRP HZ2	2757.0 e
	HE3	59 TRP HH2	1894.0 e
	HE3	60 LYS+ HN	1697.0 e
	HE3	63 THR HB	159.0 e
	HE3	63 THR QG2	1054.0 e
	HE3	64 LEU HN	7301.0 e
	HE3	64 LEU HA	3323.0 e
	HE3	64 LEU HB3	1457.0 e
	HE3	64 LEU HG	20900.0 e
	HE3	64 LEU QD1	18190.0 e
	HE3	64 LEU QD2	10590.0 e
	HE3	67 TYR HB2	1191.0 e
	HE3	74 TYR CG	243.0*2e
	HE1	59 TRP HZ2	14290.0 e
	HE1	59 TRP HH2	1544.0 e
	HE1	64 LEU QD1	153.0 e
	HE1	64 LEU QD2	1175.0 e
	HZ3	59 TRP HZ2	4378.0 e
	HZ3	59 TRP HH2	21700.0 e
	HZ3	63 THR HB	1642.0 e
	HZ3	63 THR QG2	617.0 e
	HZ3	64 LEU HN	1071.0 e
	HZ3	64 LEU HA	9584.0 e
	HZ3	64 LEU HB2	224.0 e
	HZ3	64 LEU HB3	706.0 e
	HZ3	64 LEU HG	3905.0 e
	HZ3	64 LEU QD1	15180.0 e
	HZ3	64 LEU QD2	3079.0 e
	HZ3	67 TYR HN	4585.0 e
	HZ3	67 TYR HA	1960.0 e
	HZ3	67 TYR HB2	11120.0 e
	HZ3	67 TYR HB3	8209.0 e
	HZ3	68 LEU HN	999.0 e
	HZ3	68 LEU HG	664.0 e
	HZ3	68 LEU QD2	587.0 e
	HZ3	74 TYR CG	1390.5*2e
	HZ3	74 TYR CZ	3029.5*2e
	HZ2	59 TRP HH2	34620.0 e
	HZ2	64 LEU QD1	102.0 e
	HZ2	75 ILE QD1	3137.0 e
	HH2	64 LEU HA	1857.0 e
	HH2	64 LEU QD1	3084.0 e
	HH2	67 TYR HN	1073.0 e
	HH2	67 TYR HA	858.0 e
	HH2	67 TYR HB2	5934.0 e
	HH2	67 TYR HB3	2385.0 e
	HH2	68 LEU QD2	240.0 e
	HH2	74 TYR CG	4124.0*2e
	HH2	74 TYR CZ	2992.5*2e
	HH2	75 ILE QG2	285.0 e
	HH2	75 ILE QD1	9928.0 e
60 LYS+			
	HN	60 LYS+ HA	1193.0 e
	HN	60 LYS+ QB	329.0*2e
	HN	60 LYS+ QG	3822.0*2e
	HN	60 LYS+ QD	1606.0*2e
	HN	61 GLU- HN	325.0 e
	HN	61 GLU- HA	191.0 e
	HN	62 GLU- HG2	898.0 e
	HN	63 THR HN	1148.0 e
	HN	64 LEU HN	3505.0 e
	HA	60 LYS+ QB	8250.0*2e
	HA	60 LYS+ QG	747.0*2e
	HA	60 LYS+ QE	7905.0*2e
	HA	61 GLU- HN	10950.0 e
	HA	61 GLU- HA	2869.0 e
	HA	61 GLU- QB	1654.5*2e
	HA	61 GLU- QG	1247.0*2e
	HA	62 GLU- HN	658.0 e
	HA	63 THR HN	528.0 e
	HA	64 LEU QD1	307.0 e
	HA	64 LEU QD2	3577.0 e
	QB	60 LYS+ QG	1751.2*4e
	QB	60 LYS+ QD	6575.0*4e
	QB	61 GLU- HN	13430.0*2e
	QB	62 GLU- HN	10995.0*2e
	QB	63 THR HN	4281.5*2e
	QG	60 LYS+ QE	2727.5*4e
	QG	61 GLU- HN	1802.5*2e
	QG	62 GLU- HN	5180.0*2e
	QG	62 GLU- HG3	3830.5*2e
	QG	63 THR HN	1921.5*2e
	QG	64 LEU HN	1259.0*2e
	QD	60 LYS+ QE	1118.5*4e
	QD	61 GLU- HN	1239.0*2e
	QD	62 GLU- HN	1885.5*2e
	QD	62 GLU- HG3	2539.5*2e
	QD	63 THR HN	2463.0*2e
61 GLU-			
	HN	61 GLU- HA	9962.0 e
	HN	61 GLU- QB	7190.0*2e
	HN	61 GLU- QG	2802.5*2e
	HN	62 GLU- HN	5199.0 e
	HN	62 GLU- HA	194.0 e
	HN	62 GLU- HG2	10960.0 e
	HN	63 THR HN	422.0 e
	HN	64 LEU HN	227.0 e
	HN	64 LEU HB3	594.0 e
	HN	64 LEU QD1	442.0 e
	HN	64 LEU QD2	1659.0 e
	HN	65 MET HN	175.0 e
	HN	95 ILE HG13	2254.0 e
	HN	99 LYS+ QD	37.0*2e
	HA	61 GLU- QG	11125.0*2e
	HA	62 GLU- HN	5094.0 e

HA 63 THR HN 1600.0 e
HA 64 LEU HN 1992.0 e
HA 64 LEU HB2 2933.0 e
HA 64 LEU HB3 29120.0 e
HA 64 LEU HG 146.0 e
HA 64 LEU QD1 4132.0 e
HA 95 ILE HG12 602.0 e
HA 95 ILE HG13 20260.0 e
HA 95 ILE QD1 3294.0 e
QB 61 GLU- QG 9655.0*4e
QB 62 GLU- HN 5985.0*2e
QB 99 LYS+ QG 876.2*4e
QG 62 GLU- HN 1666.5*2e
QG 95 ILE HG13 7050.0*2e
QG 95 ILE QD1 452.0*2e

62 GLU-
HN 62 GLU- HA 15170.0 e
HN 62 GLU- HB3 31850.0 e
HN 62 GLU- HG2 5907.0 e
HN 62 GLU- HG3 7086.0 e
HN 63 THR HN 7800.0 e
HN 64 LEU HN 1056.0 e
HN 65 MET HN 906.0 e
HA 62 GLU- HB2 29610.0 e
HA 62 GLU- HB3 15040.0 e
HA 62 GLU- HG2 5811.0 e
HA 62 GLU- HG3 6107.0 e
HA 63 THR HN 2429.0 e
HA 64 LEU HN 1619.0 e
HA 65 MET HN 1924.0 e
HA 66 GLU- HN 377.0 e
HB2 63 THR HN 7830.0 e
HB3 63 THR HN 3148.0 e
HG2 63 THR HN 3167.0 e
HG2 64 LEU HN 232.0 e
HG3 63 THR HN 2588.0 e
HG3 63 THR QG2 4033.0 e

63 THR
HN 63 THR HA 5610.0 e
HN 63 THR HB 398.0 e
HN 63 THR QG2 17210.0 e
HN 64 LEU HN 12210.0 e
HN 64 LEU HB3 446.0 e
HN 64 LEU QD1 483.0 e
HN 64 LEU QD2 644.0 e
HN 65 MET HN 2075.0 e
HA 63 THR QG2 17870.0 e
HA 64 LEU HN 1499.0 e
HA 64 LEU QD1 49.0 e
HA 65 MET HN 391.0 e
HA 66 GLU- HN 2863.0 e
HA 66 GLU- HB2 4222.0 e
HA 66 GLU- HB3 2251.0 e
HA 74 TYR CZ 111.0*2e
HB 63 THR QG2 7572.0 e
HB 64 LEU HN 223.0 e
HB 64 LEU QD1 165.0 e
HB 74 TYR CZ 433.0*2e
QG2 64 LEU HN 3063.0 e
QG2 74 TYR CZ 743.5*2e

64 LEU
HN 64 LEU HA 5768.0 e
HN 64 LEU HB2 12230.0 e
HN 64 LEU HB3 13070.0 e
HN 64 LEU HG 11560.0 e
HN 64 LEU QD1 9149.0 e
HN 64 LEU QD2 9086.0 e
HN 65 MET HN 12930.0 e
HN 65 MET HB3 2010.0 e
HN 66 GLU- HN 520.0 e
HN 68 LEU QD2 271.0 e
HA 64 LEU HB2 3996.0 e
HA 64 LEU HB3 14900.0 e
HA 64 LEU HG 17640.0 e
HA 64 LEU QD1 46020.0 e
HA 64 LEU QD2 8680.0 e
HA 65 MET HN 1560.0 e
HA 66 GLU- HN 293.0 e
HA 67 TYR HB2 1582.0 e
HA 67 TYR HB3 1906.0 e
HA 68 LEU HN 4020.0 e
HA 68 LEU HG 880.0 e
HA 68 LEU QD1 2054.0 e
HA 68 LEU QD2 2178.0 e
HB2 64 LEU QD1 17920.0 e
HB2 64 LEU QD2 29320.0 e
HB2 65 MET HN 9949.0 e
HB2 68 LEU QD1 2583.0 e
HB2 95 ILE QD1 1702.0 e
HB3 64 LEU HG 25420.0 e
HB3 64 LEU QD1 26030.0 e
HB3 64 LEU QD2 44050.0 e
HB3 65 MET HN 28840.0 e
HB3 66 GLU- HN 1249.0 e
HB3 68 LEU HN 861.0 e
HB3 68 LEU QD1 27860.0 e
HB3 68 LEU QD2 9959.0 e
HG 64 LEU QD1 43750.0 e
HG 64 LEU QD2 47920.0 e
QD1 65 MET HN 2234.0 e
QD1 66 GLU- HN 1061.0 e
QD1 67 TYR HA 763.0 e
QD1 67 TYR HB2 2502.0 e
QD1 67 TYR HB3 6167.0 e
QD1 94 LEU HG 2367.0 e
QD1 94 LEU QD1 1838.0 e
QD1 95 ILE QD1 2687.0 e
QD2 65 MET HN 3494.0 e
QD2 68 LEU HN 1665.0 e
QD2 95 ILE HN 869.0 e
QD2 95 ILE HA 1745.0 e
QD2 95 ILE QD1 4440.0 e
QD2 98 LEU HN 1828.0 e
QD2 99 LYS+ HN 698.0 e

65 MET
HN 65 MET HA 16100.0 e
HN 65 MET HB2 32950.0 e
HN 65 MET HB3 17300.0 e
HN 66 GLU- HN 6904.0 e
HN 68 LEU QD1 2025.0 e
HN 68 LEU QD2 760.0 e
HN 95 ILE HG13 1213.0 e
HA 65 MET HB2 8834.0 e
HA 66 GLU- HN 3042.0 e

HA 66 GLU- HG2 2877.0 e
HA 68 LEU HN 298.0 e
HA 68 LEU HB2 283.0 e
HA 68 LEU QD2 2184.0 e
66 GLU-
HN 66 GLU- HA 14930.0 e
HN 66 GLU- HB2 14190.0 e
HN 66 GLU- HB3 17350.0 e
HN 66 GLU- HG2 10120.0 e
HN 66 GLU- HG3 8288.0 e
HN 67 TYR HN 7372.0 e
HN 67 TYR HA 996.0 e
HN 67 TYR HB2 308.0 e
HN 67 TYR HB3 89.0 e
HN 74 TYR CG 212.5*2e
HA 66 GLU- HB2 23120.0 e
HA 66 GLU- HB3 34860.0 e
HA 66 GLU- HG2 8416.0 e
HA 66 GLU- HG3 22750.0 e
HA 69 GLU- HN 3592.0 e
HB2 66 GLU- HG3 26830.0 e
HB2 74 TYR CG 1759.5*2e
HB2 74 TYR CZ 603.0*2e
HB3 66 GLU- HG3 6862.0 e
HB3 74 TYR CG 1346.5*2e
HB3 74 TYR CZ 4159.5*2e
67 TYR
HN 67 TYR HA 3719.0 e
HN 67 TYR HB2 14070.0 e
HN 67 TYR HB3 14150.0 e
HN 74 TYR CG 741.5*2e
HA 67 TYR HB2 3475.0 e
HA 67 TYR HB3 2319.0 e
HA 68 LEU HN 438.0 e
HA 69 GLU- HN 748.0 e
HA 70 ASN HN 308.0 e
HA 71 PRO HA 871.0 e
HA 74 TYR QB 1716.5*2e
HA 74 TYR CG 1807.5*2e
HB2 68 LEU HN 2929.0 e
HB2 68 LEU QD2 858.0 e
HB2 74 TYR QB 229.5*2e
HB2 74 TYR CG 2124.5*2e
HB2 74 TYR CZ 251.5*2e
HB3 68 LEU QD2 3249.0 e
HB3 74 TYR CG 562.0*2e
HB3 74 TYR CZ 127.5*2e
68 LEU
HN 68 LEU HA 17870.0 e
HN 68 LEU HB2 13820.0 e
HN 68 LEU HB3 12640.0 e
HN 68 LEU HG 23250.0 e
HN 68 LEU QD1 25110.0 e
HN 68 LEU QD2 18290.0 e
HN 69 GLU- HN 8444.0 e
HA 68 LEU HB2 7426.0 e
HA 68 LEU HB3 19700.0 e
HA 68 LEU HG 7998.0 e
HA 68 LEU QD1 12510.0 e
HA 68 LEU QD2 67550.0 e
HA 69 GLU- HN 795.0 e
HA 70 ASN HN 1391.0 e
HA 82 PHE CZ 703.5*2e
HA 82 PHE HZ 103.0 e
HA 85 ILE QD1 622.0 e
HA 94 LEU QD2 223.0 e
HB2 68 LEU QD1 26350.0 e
HB2 68 LEU QD2 17620.0 e
HB2 69 GLU- HN 1369.0 e
HB2 85 ILE HG12 7699.0 e
HB3 68 LEU HG 8326.0 e
HB3 68 LEU QD1 31770.0 e
HB3 68 LEU QD2 27510.0 e
HB3 69 GLU- HN 589.0 e
HB3 82 PHE HZ 222.0 e
HG 68 LEU QD1 55760.0 e
HG 68 LEU QD2 56650.0 e
QD1 69 GLU- HN 6653.0 e
QD1 82 PHE CG 204.0*2e
QD1 82 PHE CZ 249.0*2e
QD1 82 PHE HZ 432.0 e
QD1 85 ILE HB 2088.0 e
QD1 85 ILE QG2 7526.0 e
QD1 85 ILE QD1 10250.0 e
QD1 90 GLU- HN 238.0 e
QD1 91 ARG+ HN 429.0 e
QD1 91 ARG+ HA 3947.0 e
QD1 94 LEU HN 951.0 e
QD1 94 LEU HB2 5950.0 e
QD1 94 LEU HB3 2910.0 e
QD1 94 LEU QD1 6145.0 e
QD1 94 LEU QD2 40420.0 e
QD1 95 ILE HN 3352.0 e
QD1 95 ILE HA 1522.0 e
QD1 95 ILE HG12 9329.0 e
QD1 95 ILE QD1 5605.0 e
QD1 98 LEU QD1 4546.0 e
QD2 71 PRO HA 419.0 e
QD2 71 PRO HG3 4994.0 e
QD2 82 PHE CG 852.5*2e
QD2 82 PHE CZ 2339.5*2e
QD2 82 PHE HZ 1674.0 e
QD2 85 ILE HN 700.0 e
QD2 85 ILE HB 3005.0 e
QD2 85 ILE QG2 6600.0 e
QD2 85 ILE HG13 2753.0 e
QD2 85 ILE QD1 18100.0 e
QD2 91 ARG+ HA 500.0 e
QD2 94 LEU HN 360.0 e
QD2 94 LEU HB2 435.0 e
QD2 94 LEU HB3 1696.0 e
QD2 94 LEU QD1 3378.0 e
QD2 94 LEU QD2 18640.0 e
QD2 95 ILE HN 836.0 e
QD2 98 LEU QD1 4303.0 e
69 GLU-
HN 69 GLU- HA 7993.0 e
HN 69 GLU- HB2 10260.0 e
HN 69 GLU- HB3 20490.0 e
HN 70 ASN HN 4385.0 e
HA 70 ASN HN 2331.0 e
HB2 70 ASN HN 3821.0 e
HB2 87 LYS+ HA 6035.0 e
HB3 70 ASN HN 4764.0 e

	HB3	87 LYS+	HA	982.0 e
70 ASN				
	HN	70 ASN	HB2	4143.0 e
	HN	70 ASN	HB3	3932.0 e
	HN	71 PRO	HD2	76.0 e
	HN	71 PRO	HD3	2627.0 e
	HB2	73 LYS+	HN	194.0 e
71 PRO				
	HA	71 PRO	HG2	2908.0 e
	HA	71 PRO	HG3	3835.0 e
	HA	71 PRO	HD3	68.0 e
	HA	72 LYS+	HN	1492.0 e
	HA	73 LYS+	HN	564.0 e
	HA	74 TYR	HN	1010.0 e
	HA	74 TYR	CG	333.0*2e
	HA	75 ILE	HN	129.0 e
	HA	76 PRO	HB3	305.0 e
	HG2	71 PRO	HD2	565.0 e
	HG2	71 PRO	HD3	757.0 e
	HG2	72 LYS+	HN	761.0 e
	HG2	76 PRO	HB3	795.0 e
	HG2	82 PHE	CG	2876.5*2e
	HG2	82 PHE	CZ	800.0*2e
	HD2	72 LYS+	HN	412.0 e
	HD3	82 PHE	HZ	583.0 e
72 LYS+				
	HN	72 LYS+	HA	6841.0 e
	HN	72 LYS+	HB2	11300.0 e
	HN	72 LYS+	HB3	14420.0 e
	HN	72 LYS+	HG2	16300.0 e
	HN	72 LYS+	HG3	1862.0 e
	HN	73 LYS+	HN	9427.0 e
	HA	72 LYS+	HB2	12200.0 e
	HA	72 LYS+	HB3	16310.0 e
	HA	72 LYS+	HG2	16370.0 e
	HA	72 LYS+	HG3	412.0 e
	HA	73 LYS+	HN	1784.0 e
	HA	73 LYS+	HB2	87.0 e
	HA	76 PRO	HB3	55.0 e
	HA	76 PRO	HG2	642.0 e
	HB2	72 LYS+	HG2	26690.0 e
	HB2	72 LYS+	HG3	8916.0 e
	HB2	73 LYS+	HN	1401.0 e
	HB3	72 LYS+	HG2	41600.0 e
	HB3	72 LYS+	HG3	6918.0 e
	HB3	73 LYS+	HN	2313.0 e
	HB3	76 PRO	HA	589.0 e
	HG2	73 LYS+	HN	2920.0 e
	HG2	76 PRO	HA	2460.0 e
	HG2	76 PRO	HG3	535.0 e
	HG3	73 LYS+	HN	714.0 e
	HG3	76 PRO	HA	482.0 e
73 LYS+				
	HN	73 LYS+	HA	12000.0 e
	HN	73 LYS+	HB2	16440.0 e
	HN	73 LYS+	HB3	14980.0 e
	HN	73 LYS+	QG	1137.5*2e
	HN	73 LYS+	QD	1179.0*2e
	HN	73 LYS+	QE	80.5*2e
	HN	74 TYR	HN	17490.0 e
	HN	74 TYR	QB	966.0*2e
	HA	73 LYS+	HB2	6671.0 e
	HA	73 LYS+	HB3	4335.0 e
	HA	73 LYS+	QG	5700.0*2e
	HA	73 LYS+	QD	2108.0*2e
	HA	73 LYS+	QE	174.0*2e
	HA	74 TYR	HN	40.0 e
	HA	76 PRO	HG3	988.0 e
	HB2	74 TYR	HN	2194.0 e
	HB3	74 TYR	HN	2010.0 e
	QG	73 LYS+	QE	2398.2*4e
74 TYR				
	HN	74 TYR	QB	19270.0*2e
	HN	74 TYR	CG	1382.0*2e
	HN	75 ILE	HN	5573.0 e
	HN	76 PRO	HB3	1850.0 e
	QB	75 ILE	HN	392.0*2e
	QB	75 ILE	QG2	693.5*2e
	CG	74 TYR	CZ	12287.5*4e
	CG	75 ILE	HN	1071.5*2e
	CG	75 ILE	QG2	759.5*2e
	CG	76 PRO	QD	70.2*4e
75 ILE				
	HN	75 ILE	HB	4698.0 e
	HN	75 ILE	QG2	1667.0 e
	HN	75 ILE	QD1	4791.0 e
	HN	78 THR	HB	317.0 e
	HB	75 ILE	QG2	17290.0 e
	HB	75 ILE	QD1	6768.0 e
	HB	78 THR	HB	5438.0 e
	QG2	75 ILE	QD1	47900.0 e
	QG2	77 GLY	HA2	3591.0 e
	QG2	78 THR	HN	3290.0 e
	QG2	78 THR	HA	1760.0 e
	QG2	78 THR	HB	14990.0 e
	QG2	78 THR	QG2	3981.0 e
76 PRO				
	HA	76 PRO	HB2	13210.0 e
	HA	76 PRO	HB3	6415.0 e
	HA	76 PRO	HG2	6289.0 e
	HA	76 PRO	HG3	256.0 e
	HA	76 PRO	QD	53.5*2e
	HA	77 GLY	HN	3466.0 e
	HB2	76 PRO	HG2	11980.0 e
	HB2	76 PRO	HG3	234.0 e
	HB2	77 GLY	HN	2288.0 e
	HB2	78 THR	HN	498.0 e
	HB3	77 GLY	HN	132.0 e
	HG2	76 PRO	QD	5465.0*2e
	HG2	77 GLY	HN	782.0 e
77 GLY				
	HN	77 GLY	HA1	124.0 e
	HN	77 GLY	HA2	1629.0 e
	HN	78 THR	HN	5647.0 e
	HN	78 THR	QG2	2291.0 e
	HA1	78 THR	HN	237.0 e
78 THR				
	HN	78 THR	HA	5284.0 e
	HN	78 THR	HB	14390.0 e
	HN	78 THR	QG2	25650.0 e
	HN	78 THR	HG1	321.0 e
	HN	81 ILE	QG2	77.0 e
	HA	78 THR	HB	4701.0 e
	HA	78 THR	QG2	9022.0 e

HA 78 THR HG1 2987.0 e
HA 79 LYS+ HN 6144.0 e
HA 79 LYS+ HG2 725.0 e
HA 79 LYS+ HG3 468.0 e
HB 78 THR QG2 31870.0 e
HB 79 LYS+ HN 1482.0 e
QG2 78 THR HG1 1250.0 e
QG2 80 MET HN 19330.0 e
QG2 80 MET HB2 5465.0 e
HG1 79 LYS+ HN 3408.0 e
HG1 80 MET HN 695.0 e

79 LYS+

HN 79 LYS+ HG2 1801.0 e
HN 79 LYS+ HG3 3191.0 e
HN 80 MET HN 5433.0 e
HG2 79 LYS+ QE 1576.5*2e
HG3 79 LYS+ QE 178.5*2e

80 MET

HN 80 MET HA 1135.0 e
HN 80 MET HB2 2813.0 e
HA 80 MET HB2 1827.0 e
HA 80 MET HB3 8389.0 e
HA 81 ILE HN 6219.0 e

81 ILE

HN 81 ILE HA 2182.0 e
HN 81 ILE HB 14250.0 e
HN 81 ILE QG2 9323.0 e
HN 81 ILE HG12 12380.0 e
HN 81 ILE HG13 4684.0 e
HN 81 ILE QD1 5371.0 e
HA 81 ILE HB 3392.0 e
HA 81 ILE QG2 15670.0 e
HA 81 ILE HG12 4431.0 e
HA 81 ILE HG13 1991.0 e
HA 81 ILE QD1 12680.0 e
HA 82 PHE HN 6131.0 e
HB 81 ILE QG2 58830.0 e
HB 81 ILE HG12 21780.0 e
HB 81 ILE HG13 36870.0 e
HB 81 ILE QD1 32860.0 e
HB 82 PHE HN 227.0 e
QG2 81 ILE HG13 32710.0 e
QG2 81 ILE QD1 110500.0 e
QG2 82 PHE HN 4483.0 e
QG2 82 PHE HA 620.0 e
HG12 81 ILE QD1 83380.0 e
HG12 82 PHE HN 79.0 e
HG13 81 ILE QD1 47600.0 e
QD1 82 PHE HN 1277.0 e

82 PHE

HN 82 PHE HA 1505.0 e
HN 82 PHE QB 490.5*2e
HN 83 ALA HA 304.0 e
HA 82 PHE QB 131.0*2e
HA 82 PHE CG 3679.5*2e
HA 82 PHE CZ 1321.5*2e
QB 82 PHE CG 1484.2*4e
QB 82 PHE CZ 539.8*4e
CG 82 PHE HZ 4424.0*2e
CG 85 ILE HB 439.0*2e
CG 85 ILE HG12 2059.0*2e
CZ 82 PHE HZ 16630.0*2e
CZ 84 GLY HN 135.0*2e
CZ 84 GLY HA1 633.0*2e
CZ 84 GLY HA2 547.5*2e
CZ 85 ILE HN 1473.0*2e
CZ 85 ILE HA 2928.5*2e
CZ 85 ILE HB 7735.0*2e
CZ 85 ILE QG2 1828.0*2e
CZ 85 ILE HG12 9455.0*2e
CZ 85 ILE HG13 7575.0*2e
CZ 85 ILE QD1 6910.0*2e
HZ 84 GLY HN 457.0 e
HZ 84 GLY HA1 2516.0 e
HZ 84 GLY HA2 1006.0 e
HZ 85 ILE HN 1009.0 e
HZ 85 ILE HA 4296.0 e
HZ 85 ILE HB 12660.0 e
HZ 85 ILE QG2 8573.0 e
HZ 85 ILE HG12 22830.0 e
HZ 85 ILE HG13 20490.0 e
HZ 85 ILE QD1 20850.0 e

83 ALA

HN 83 ALA HA 226.0 e
HN 83 ALA QB 7079.0 e
HA 83 ALA QB 73870.0 e
QB 84 GLY HN 2346.0 e
QB 84 GLY HA1 3459.0 e
QB 84 GLY HA2 388.0 e

84 GLY

HN 84 GLY HA1 1315.0 e
HA1 85 ILE HG13 5933.0 e
HA1 85 ILE QD1 1587.0 e
HA2 85 ILE HG13 319.0 e

85 ILE

HN 85 ILE HA 12630.0 e
HN 85 ILE HB 6414.0 e
HN 85 ILE QG2 5657.0 e
HN 85 ILE HG12 4909.0 e
HN 85 ILE HG13 3482.0 e
HN 85 ILE QD1 6702.0 e
HN 86 LYS+ HN 1441.0 e
HA 85 ILE HB 8870.0 e
HA 85 ILE QG2 33860.0 e
HA 85 ILE HG12 11830.0 e
HA 85 ILE HG13 20350.0 e
HA 85 ILE QD1 12020.0 e
HA 86 LYS+ HN 22660.0 e
HB 85 ILE QG2 43610.0 e
HB 85 ILE HG13 11440.0 e
HB 85 ILE QD1 30990.0 e
QG2 85 ILE HG13 45050.0 e
QG2 85 ILE QD1 72430.0 e
QG2 86 LYS+ HN 7811.0 e
QG2 86 LYS+ HA 2933.0 e
QG2 86 LYS+ HB2 21530.0 e
QG2 86 LYS+ QG 1622.0*2e
QG2 87 LYS+ HN 12290.0 e
QG2 90 GLU- HN 3638.0 e
QG2 90 GLU- HA 2550.0 e
QG2 90 GLU- HB2 10280.0 e
QG2 90 GLU- HB3 7398.0 e
QG2 91 ARG+ HN 4347.0 e
QG2 91 ARG+ HA 5743.0 e

	HG12	85 ILE QD1	37450.0 e
	HG13	85 ILE QD1	59460.0 e
	HG13	86 LYS+ HN	5993.0 e
	HG13	86 LYS+ QG	335.5*2e
	HG13	90 GLU- HA	1041.0 e
	QD1	86 LYS+ HN	1900.0 e
	QD1	86 LYS+ QG	668.5*2e
	QD1	90 GLU- HB2	295.0 e
	QD1	90 GLU- HB3	4419.0 e
	QD1	94 LEU HB2	961.0 e
	QD1	94 LEU HB3	19790.0 e
	QD1	94 LEU QD1	7803.0 e
86 LYS+			
	HN	86 LYS+ HA	7730.0 e
	HN	86 LYS+ HB2	5078.0 e
	HN	86 LYS+ HB3	10320.0 e
	HN	86 LYS+ QG	2218.0*2e
	HN	86 LYS+ QD	1818.5*2e
	HN	90 GLU- HN	298.0 e
	HN	90 GLU- HB2	6034.0 e
	HN	90 GLU- HB3	2180.0 e
	HA	86 LYS+ HB2	20180.0 e
	HA	86 LYS+ HB3	20550.0 e
	HA	86 LYS+ QG	5630.0*2e
	HA	86 LYS+ QD	3243.5*2e
	HA	86 LYS+ HE2	3121.0 e
	HA	86 LYS+ HE3	1028.0 e
	HA	87 LYS+ HN	9743.0 e
	HB2	86 LYS+ HE2	710.0 e
	HB2	87 LYS+ HN	8485.0 e
	HB2	88 LYS+ HN	1527.0 e
	HB2	89 THR HN	6315.0 e
	HB2	90 GLU- HN	6100.0 e
	HB3	87 LYS+ HN	36120.0 e
	HB3	87 LYS+ HA	1385.0 e
	HB3	88 LYS+ HN	2264.0 e
	HB3	90 GLU- HN	4436.0 e
	QG	87 LYS+ HN	4868.5*2e
	QD	89 THR HB	1918.0*2e
	HE2	89 THR QG2	7462.0 e
87 LYS+			
	HN	87 LYS+ HA	3662.0 e
	HN	87 LYS+ QB	22560.0*2e
	HN	88 LYS+ HN	407.0 e
	HN	88 LYS+ QB	2451.5*2e
	HN	89 THR HN	2486.0 e
	HN	90 GLU- HN	3870.0 e
	HN	90 GLU- HB3	3207.0 e
	HA	88 LYS+ HN	6588.0 e
	HA	89 THR HN	638.0 e
	QB	88 LYS+ HN	304.5*2e
	QB	90 GLU- HN	2313.0*2e
88 LYS+			
	HN	88 LYS+ HA	2421.0 e
	HN	88 LYS+ QB	5760.0*2e
	HN	88 LYS+ QG	75.0*2e
	HN	88 LYS+ QD	1037.0*2e
	HN	88 LYS+ QE	225.5*2e
	HN	89 THR HN	2470.0 e
	HN	89 THR HA	275.0 e
	HA	88 LYS+ QB	23805.0*2e
	HA	88 LYS+ QG	367.5*2e
	HA	88 LYS+ QD	11885.0*2e
	HA	88 LYS+ QE	2587.0*2e
	HA	89 THR HN	1971.0 e
	HA	91 ARG+ HN	2157.0 e
	QB	89 THR HN	1860.0*2e
	QG	89 THR HA	243.0*2e
89 THR			
	HN	89 THR HA	12130.0 e
	HN	89 THR HB	9024.0 e
	HN	89 THR QG2	20690.0 e
	HN	90 GLU- HN	3553.0 e
	HA	89 THR HB	29400.0 e
	HA	89 THR QG2	74650.0 e
	HA	90 GLU- HN	2251.0 e
	HA	90 GLU- QG	2950.5*2e
	HA	92 GLU- HN	4397.0 e
	HB	89 THR QG2	115500.0 e
	HB	90 GLU- HN	3423.0 e
	QG2	90 GLU- HN	2503.0 e
	QG2	93 ASP- HN	1819.0 e
90 GLU-			
	HN	90 GLU- HA	7329.0 e
	HN	90 GLU- HB2	14820.0 e
	HN	90 GLU- HB3	16820.0 e
	HN	90 GLU- QG	10100.0*2e
	HN	91 ARG+ HN	7734.0 e
	HA	90 GLU- HB2	12280.0 e
	HA	90 GLU- HB3	20380.0 e
	HA	90 GLU- QG	5270.0*2e
	HA	91 ARG+ HN	2169.0 e
	HA	93 ASP- QB	2228.5*2e
	HB3	91 ARG+ HN	4428.0 e
	QG	91 ARG+ HN	464.0*2e
	QG	92 GLU- HN	2833.5*2e
91 ARG+			
	HN	91 ARG+ HA	16190.0 e
	HN	91 ARG+ HB2	8678.0 e
	HN	91 ARG+ HB3	23560.0 e
	HN	92 GLU- HN	11290.0 e
	HA	91 ARG+ HB2	16840.0 e
	HA	91 ARG+ HB3	16940.0 e
	HA	92 GLU- HN	2127.0 e
	HA	92 GLU- HA	1167.0 e
	HA	94 LEU HN	2346.0 e
	HA	94 LEU QD2	7197.0 e
	HA	95 ILE QD1	850.0 e
92 GLU-			
	HN	92 GLU- HA	18790.0 e
	HN	92 GLU- QB	10040.0*2e
	HN	92 GLU- QG	5910.0*2e
	HA	92 GLU- QB	12350.0*2e
	HA	95 ILE HN	2412.0 e
	HA	95 ILE HA	356.0 e
	HA	95 ILE QG2	11300.0 e
	HA	95 ILE HG13	3468.0 e
	HA	95 ILE QD1	1950.0 e
	HA	96 ALA HN	2579.0 e
	QG	95 ILE QG2	3065.5*2e
93 ASP-			
	HN	93 ASP- HA	11740.0 e
	HN	93 ASP- QB	14575.0*2e
	HN	94 LEU HN	19460.0 e

HN 94 LEU HB2 7784.0 e
HN 95 ILE HN 3585.0 e
HN 96 ALA HN 1595.0 e
HN 96 ALA QB 2508.0 e
HA 93 ASP- QB 13950.0*2e
HA 94 LEU HN 7679.0 e
HA 96 ALA HN 1417.0 e
QB 94 LEU HN 9935.0*2e

94 LEU
HN 94 LEU HA 16030.0 e
HN 94 LEU HB2 23960.0 e
HN 94 LEU HB3 37400.0 e
HN 94 LEU HG 4392.0 e
HN 94 LEU QD1 10760.0 e
HN 94 LEU QD2 8849.0 e
HN 95 ILE HN 21180.0 e
HN 95 ILE QG2 355.0 e
HN 98 LEU QD1 500.0 e
HA 94 LEU HB2 8734.0 e
HA 94 LEU HB3 10290.0 e
HA 94 LEU HG 2482.0 e
HA 94 LEU QD1 29410.0 e
HA 94 LEU QD2 8806.0 e
HA 95 ILE HN 3677.0 e
HA 96 ALA HN 2815.0 e
HA 97 TYR HD1 730.0 e
HB2 94 LEU HG 6002.0 e
HB2 94 LEU QD1 35650.0 e
HB2 94 LEU QD2 42940.0 e
HB2 95 ILE HN 3033.0 e
HB2 97 TYR HD1 401.0 e
HB3 94 LEU HG 2363.0 e
HB3 94 LEU QD1 28340.0 e
HB3 94 LEU QD2 20980.0 e
HB3 95 ILE HN 7694.0 e
HG 94 LEU QD2 50560.0 e
HG 95 ILE HN 2675.0 e
HG 95 ILE HA 463.0 e
HG 98 LEU QD1 8167.0 e
QD1 95 ILE HN 6167.0 e
QD1 96 ALA HN 202.0 e
QD1 97 TYR HD1 14480.0 e
QD1 97 TYR HE1 1950.0 e
QD1 98 LEU HN 5240.0 e
QD1 98 LEU QD1 18980.0 e
QD1 99 LYS+ HN 1078.0 e
QD2 95 ILE HN 3578.0 e
QD2 95 ILE HA 861.0 e
QD2 95 ILE QD1 263.0 e
QD2 96 ALA HN 131.0 e
QD2 97 TYR HD1 1006.0 e
QD2 98 LEU HN 607.0 e
QD2 98 LEU HG 6005.0 e
QD2 98 LEU QD1 34840.0 e

95 ILE
HN 95 ILE HA 12740.0 e
HN 95 ILE HB 34940.0 e
HN 95 ILE QG2 11240.0 e
HN 95 ILE HG12 21110.0 e
HN 95 ILE HG13 9127.0 e
HN 95 ILE QD1 10320.0 e
HN 96 ALA HN 17950.0 e
HN 96 ALA HA 1346.0 e
HN 98 LEU QD1 622.0 e
HA 95 ILE HB 12910.0 e
HA 95 ILE QG2 6259.0 e
HA 95 ILE HG12 16220.0 e
HA 95 ILE HG13 18300.0 e
HA 95 ILE QD1 15920.0 e
HA 96 ALA HN 4543.0 e
HA 97 TYR HN 779.0 e
HA 98 LEU HN 6494.0 e
HA 98 LEU HB2 5409.0 e
HA 98 LEU HB3 1733.0 e
HA 98 LEU QD1 31000.0 e
HA 98 LEU QD2 2328.0 e
HA 99 LYS+ HN 1788.0 e
HB 95 ILE QG2 20720.0 e
HB 95 ILE HG13 21340.0 e
HB 95 ILE QD1 .0 e
HB 96 ALA HN 12900.0 e
QG2 95 ILE HG12 21220.0 e
QG2 95 ILE HG13 32920.0 e
QG2 95 ILE QD1 37970.0 e
QG2 96 ALA HN 1562.0 e
HG12 95 ILE QD1 24920.0 e
HG12 98 LEU QD1 2235.0 e
HG13 95 ILE QD1 16050.0 e
HG13 96 ALA HN 6389.0 e
HG13 96 ALA HA 2019.0 e
HG13 98 LEU QD1 743.0 e
QD1 96 ALA HN 1864.0 e
QD1 98 LEU QD1 3340.0 e

96 ALA
HN 96 ALA HA 26290.0 e
HN 96 ALA QB 68140.0 e
HN 97 TYR HN 4436.0 e
HN 98 LEU HN 2081.0 e
HN 98 LEU QD1 240.0 e
HA 96 ALA QB 45890.0 e
HA 97 TYR HN 10350.0 e
HA 99 LYS+ HN 4502.0 e
HA 99 LYS+ QB 3135.0*2e
HA 99 LYS+ QD 102.0*2e
QB 97 TYR HN 25170.0 e

97 TYR
HN 97 TYR HA 7696.0 e
HN 97 TYR HB2 22660.0 e
HN 97 TYR HB3 18210.0 e
HN 97 TYR HD1 7034.0 e
HN 97 TYR HD2 3337.0 e
HN 98 LEU HN 14560.0 e
HA 97 TYR HB2 18860.0 e
HA 97 TYR HB3 3496.0 e
HA 97 TYR HD1 5603.0 e
HA 97 TYR HD2 13020.0 e
HA 98 LEU HN 2327.0 e
HB2 97 TYR HD1 11180.0 e
HB2 97 TYR HD2 9340.0 e
HB2 97 TYR HE1 833.0 e
HB2 97 TYR HE2 237.0 e
HB2 98 LEU HN 5815.0 e
HB3 97 TYR HD1 11390.0 e
HB3 97 TYR HD2 3962.0 e

	HB3	97 TYR HE1	1247.0 e
	HB3	98 LEU HN	7615.0 e
	HD1	97 TYR HE1	14970.0 e
	HD1	97 TYR HE2	14020.0 e
	HD1	98 LEU HN	7357.0 e
	HD1	98 LEU HA	2594.0 e
	HD1	98 LEU HB3	16020.0 e
	HD1	98 LEU HG	7994.0 e
	HD1	98 LEU QD1	2906.0 e
	HD1	98 LEU QD2	11100.0 e
	HD1	99 LYS+ HN	642.0 e
	HD1	100 LYS+ HB3	1461.0 e
	HD1	101 ALA QB	2943.0 e
	HD2	97 TYR HE1	13650.0 e
	HD2	97 TYR HE2	28560.0 e
	HD2	98 LEU HN	1781.0 e
	HD2	98 LEU QD1	422.0 e
	HD2	101 ALA QB	3203.0 e
	HE1	98 LEU HN	1003.0 e
	HE1	98 LEU HA	997.0 e
	HE1	98 LEU HG	2123.0 e
	HE1	98 LEU QD1	701.0 e
	HE1	98 LEU QD2	8830.0 e
	HE1	101 ALA QB	9622.0 e
	HE2	101 ALA QB	3900.0 e
98 LEU			
	HN	98 LEU HA	13610.0 e
	HN	98 LEU HB2	15220.0 e
	HN	98 LEU HB3	43030.0 e
	HN	98 LEU HG	26910.0 e
	HN	98 LEU QD1	15120.0 e
	HN	98 LEU QD2	19040.0 e
	HN	99 LYS+ HN	29170.0 e
	HA	98 LEU HB2	11040.0 e
	HA	98 LEU HB3	19570.0 e
	HA	98 LEU HG	242.0 e
	HA	98 LEU QD1	12830.0 e
	HA	98 LEU QD2	53650.0 e
	HA	99 LYS+ HN	2664.0 e
	HA	100 LYS+ HN	310.0 e
	HA	101 ALA HN	4661.0 e
	HA	101 ALA HA	433.0 e
	HA	101 ALA QB	13270.0 e
	HA	102 THR HN	2553.0 e
	HA	102 THR QG2	6660.0 e
	HB2	98 LEU QD1	31740.0 e
	HB2	98 LEU QD2	8442.0 e
	HB2	99 LYS+ HN	21550.0 e
	HB3	98 LEU QD1	33960.0 e
	HG	98 LEU QD1	38860.0 e
	HG	98 LEU QD2	28270.0 e
	HG	100 LYS+ HN	1701.0 e
	QD1	99 LYS+ HN	3212.0 e
	QD2	99 LYS+ HN	1008.0 e
	QD2	101 ALA QB	7475.0 e
99 LYS+			
	HN	99 LYS+ HA	18720.0 e
	HN	99 LYS+ QB	12885.0*2e
	HN	99 LYS+ QG	1525.5*2e
	HN	99 LYS+ QD	2697.5*2e
	HN	100 LYS+ HN	18440.0 e
	HA	99 LYS+ QB	6560.0*2e
	HA	99 LYS+ QG	12040.0*2e
	HA	99 LYS+ QD	16530.0*2e
	HA	100 LYS+ HN	4017.0 e
	HA	102 THR HN	1136.0 e
	HA	102 THR HG1	1509.0 e
	QB	99 LYS+ QG	6180.0*4e
	QB	99 LYS+ QD	3310.0*4e
	QB	100 LYS+ HN	4516.0*2e
	QB	101 ALA HN	1375.5*2e
	QG	99 LYS+ QD	25525.0*4e
	QG	99 LYS+ HE2	1585.0*2e
	QG	99 LYS+ HE3	810.5*2e
	QG	102 THR HG1	443.0*2e
	QD	99 LYS+ HE2	2833.5*2e
	QD	99 LYS+ HE3	3834.5*2e
100 LYS+			
	HN	100 LYS+ HA	9679.0 e
	HN	100 LYS+ HB2	23460.0 e
	HN	100 LYS+ HB3	22910.0 e
	HN	100 LYS+ HG2	2638.0 e
	HN	100 LYS+ HG3	6746.0 e
	HN	100 LYS+ QE	509.0*2e
	HN	101 ALA HN	11820.0 e
	HA	100 LYS+ HB2	26440.0 e
	HA	100 LYS+ HB3	19620.0 e
	HA	100 LYS+ HG2	16950.0 e
	HA	100 LYS+ HG3	11460.0 e
	HA	100 LYS+ QE	709.0*2e
	HB2	101 ALA HN	17530.0 e
	HG2	100 LYS+ QE	12195.0*2e
	HG3	100 LYS+ QE	10845.0*2e
	HG3	101 ALA HN	2696.0 e
101 ALA			
	HN	101 ALA HA	24120.0 e
	HN	101 ALA QB	36170.0 e
	HN	102 THR HN	6633.0 e
	HA	101 ALA QB	73950.0 e
	HA	102 THR HN	4303.0 e
	HA	103 ASN HN	4365.0 e
	HA	104 GLU- HN	2378.0 e
	QB	102 THR HN	11320.0 e
102 THR			
	HN	102 THR HA	763.0 e
	HN	102 THR QG2	12200.0 e
	HN	103 ASN HN	4290.0 e
	HN	104 GLU- HN	192.0 e
	HA	102 THR QG2	3683.0 e
	HA	103 ASN HN	924.0 e
	HG1	103 ASN HB2	2535.0 e
	HG1	103 ASN HB3	1547.0 e
103 ASN			
	HN	103 ASN HB2	7208.0 e
	HN	103 ASN HB3	10380.0 e
	HN	104 GLU- HN	14050.0 e
	HN	104 GLU- HA	313.0 e
	HN	104 GLU- QG	351.0*2e
	HB2	104 GLU- HN	2549.0 e
	HB3	104 GLU- HN	4153.0 e
	HB3	104 GLU- HA	944.0 e
104 GLU-			
	HN	104 GLU- HA	10090.0 e
	HN	104 GLU- QB	8100.0*2e

HN 104 GLU- QG 5155.0*2e
HA 104 GLU- QB 13495.0*2e
HA 104 GLU- QG 5715.0*2e

Table 3: H-bond constraints

103 ASN			
	HN	101 ALA O	2.40
	N	101 ALA O	3.40
102 THR			
	HN	98 LEU O	2.40
	N	98 LEU O	3.40
101 ALA			
	HN	97 TYR O	2.40
	N	97 TYR O	3.40
100 LYS+			
	HN	97 TYR O	2.40
	N	97 TYR O	3.40
99 LYS+			
	HN	95 ILE O	2.40
	N	95 ILE O	3.40
98 LEU			
	HN	94 LEU O	2.40
	N	94 LEU O	3.40
94 LEU			
	HN	90 GLU- O	2.40
	N	90 GLU- O	3.40
93 ASP-			
	HN	89 THR O	2.40
	N	89 THR O	3.40
68 LEU			
	HN	64 LEU O	2.40
	N	64 LEU O	3.40
65 MET			
	HN	61 GLU- O	2.40
	N	61 GLU- O	3.40
64 LEU			
	HN	60 LYS+ O	2.40
	N	60 LYS+ O	3.40
14 CYSS			
	HN	11 VAL O	2.40
	N	11 VAL O	3.40
13 LYS+			
	HN	10 PHE O	2.40
	N	10 PHE O	3.40
9 ILE			
	HN	6 GLY O	2.40
	N	6 GLY O	3.40

Table 4: 1D NOE constraints

18 HEM			
	HE1	30 PRO HG3	4.00
	HE1	30 PRO HG2	4.00
	HE1	30 PRO HD3	4.00
	HE1	30 PRO HD2	4.00
	HE1	30 PRO HB2	5.50
	HE1	30 PRO HB3	5.50
	HE1	30 PRO HA	5.50
	HE1	29 GLY HA2	5.50
	HE1	18 HEM QM5	6.50
	HE1	18 HEM QM8	6.50
80 MET			
	HG2	18 HEM QM5	5.50
	HG2	82 PHE QB	5.50
	HG2	81 ILE HA	5.50
	HG2	82 PHE HA	5.50
	HG2	18 HEM QM3	6.50
	QE	68 LEU QD2	6.50
	QE	80 MET HB2	6.50
	QE	18 HEM QM1	6.50
	QE	18 HEM QM3	6.50
	QE	18 HEM QM8	6.50
67 TYR			
	HH	18 HEM HAP72	6.50
	HH	18 HEM HAP71	6.50
	HH	18 HEM HBP74	6.50
	HH	18 HEM QM8	6.50
	HH	80 MET HB2	6.50
	HH	80 MET QE	6.50
	HH	59 TRP HH2	6.50
	HH	68 LEU QD2	6.50

Table 5: Experimental pseudocontact shifts

1 GLY HN -.20	27 LYS+ HN .53	49 THR HG22 -.33
2 ASP- HN -.19	27 LYS+ HA .16	49 THR HG23 -.33
2 ASP- HA -.16	28 THR HN .01	50 ASP- HN .00
3 VAL HN -.14	28 THR HA -1.13	50 ASP- HA -.19
3 VAL HA -.21	28 THR HB -1.31	51 ALA HN .20
3 VAL HB -.12	28 THR HG21 -2.19	51 ALA HA .17
4 GLU- HN -.14	28 THR HG22 -2.19	51 ALA HB1 .27
4 GLU- HA -.09	28 THR HG23 -2.19	51 ALA HB2 .27
5 LYS+ HN -.14	29 GLY HN -.54	51 ALA HB3 .27
5 LYS+ HA -.18	30 PRO HA .09	52 ASN HN .08
6 GLY HN -.23	31 ASN HN .91	52 ASN HA .43
7 LYS+ HN -.05	31 ASN HA 1.84	53 LYS+ HN .53
7 LYS+ HA -.14	32 LEU HN 1.70	53 LYS+ HA .11
8 LYS+ HN -.15	32 LEU HA .96	54 ASN HN -.60
8 LYS+ HA -.11	32 LEU HG 1.79	54 ASN HA .24
9 ILE HN -.29	33 HIS HN .76	55 LYS+ HN -.50
9 ILE HA -.41	33 HIS HA .47	55 LYS+ HA .16
9 ILE HB -.60	34 GLY HN .09	56 GLY HN .68
9 ILE HG21 -.85	35 LEU HN .03	57 ILE HN .14
9 ILE HG22 -.85	35 LEU HA -.03	57 ILE HA .04
9 ILE HG23 -.85	35 LEU HG -.30	57 ILE HB .02
10 PHE HN -.30	36 PHE HN -.09	57 ILE HG21 .05
10 PHE HA -.69	36 PHE HA -.24	57 ILE HG22 .05
10 PHE HZ 2.52	36 PHE HZ -.43	57 ILE HG23 .05
11 VAL HN .01	37 GLY HN -.25	57 ILE HD11 .09
11 VAL HA .24	38 ARG+ HN -.22	57 ILE HD12 .09
11 VAL HB -.02	38 ARG+ HA -.14	57 ILE HD13 .09
12 GLN HN -.20	39 LYS+ HN -.13	58 THR HN .09
12 GLN HA -.15	39 LYS+ HA -.14	58 THR HA -.13
13 LYS+ HN -.57	40 THR HN .14	58 THR HB -.06
13 LYS+ HA -.75	40 THR HA -.38	58 THR HG21 -.11
15 ALA HN .65	40 THR HB -.03	58 THR HG22 -.11
15 ALA HA 2.02	40 THR HG21 -.10	58 THR HG23 -.11
15 ALA HB1 .77	40 THR HG22 -.10	59 TRP HN -.31
15 ALA HB2 .77	40 THR HG23 -.10	59 TRP HA -.20
15 ALA HB3 .77	41 GLY HN .52	59 TRP HD1 -.19
16 GLN HN 1.02	42 GLN HN -.84	59 TRP HE3 -.31
16 GLN HA .76	42 GLN HA -.16	59 TRP HE1 -.51
19 THR HN 2.83	43 ALA HN -.62	59 TRP HZ3 -.23
19 THR HA 1.70	43 ALA HA -.13	59 TRP HZ2 .48
19 THR HB 1.07	43 ALA HB1 -.16	59 TRP HH2 .55
19 THR HG21 1.09	43 ALA HB2 -.16	60 LYS+ HN -.26
19 THR HG22 1.09	43 ALA HB3 -.16	60 LYS+ HA -.21
19 THR HG23 1.09	45 GLY HN -.23	61 GLU- HN -.19
20 VAL HN 1.10	46 PHE HN -.38	61 GLU- HA -.35
20 VAL HA 1.07	46 PHE HA -.54	62 GLU- HN -.19
20 VAL HB .62	46 PHE HZ -3.07	62 GLU- HA -.17
21 GLU- HN .61	47 THR HN -.60	63 THR HN -.22
21 GLU- HA .40	47 THR HA -.56	63 THR HA -.04
22 LYS+ HN .19	47 THR HB -.68	63 THR HB -.03
22 LYS+ HA .20	47 THR HG21 -.48	63 THR HG21 -.06
23 GLY HN .18	47 THR HG22 -.48	63 THR HG22 -.06
24 GLY HN .41	47 THR HG23 -.48	63 THR HG23 -.06
25 LYS+ HN .48	48 TYR HN -.56	64 LEU HN -.42
25 LYS+ HA .29	48 TYR HA -1.21	64 LEU HA -.58
26 HIS HN .32	49 THR HN -.72	64 LEU HG -.66
26 HIS HA .55	49 THR HA -.38	65 MET HN -.36
26 HIS HD2 -.15	49 THR HB .05	65 MET HA -.38
26 HIS HE1 .07	49 THR HG21 -.33	66 GLU- HN -.16

66 GLU- HA -.01
67 TYR HN -.21
67 TYR HA .32
68 LEU HN -.26
68 LEU HA -.59
68 LEU HG -1.36
69 GLU- HN -.15
69 GLU- HA -.15
70 ASN HN .41
70 ASN HA .51
71 PRO HA 1.45
72 LYS+ HN 1.72
72 LYS+ HA 1.43
73 LYS+ HN .78
73 LYS+ HA .47
74 TYR HN .78
75 ILE HN 1.12
75 ILE HA .81
75 ILE HB 1.55
75 ILE HG21 .65
75 ILE HG22 .65
75 ILE HG23 .65
76 PRO HA .68
77 GLY HN .65
78 THR HN .89
78 THR HA .68
78 THR HB 1.64
78 THR HG21 2.70
78 THR HG22 2.70
78 THR HG23 2.70
79 LYS+ HN .26
81 ILE HN .60
81 ILE HA 1.51
81 ILE HB .03
81 ILE HG21 .29
81 ILE HG22 .29
81 ILE HG23 .29
81 ILE HD11 .17
81 ILE HD12 .17
81 ILE HD13 .17
82 PHE HN 2.42
82 PHE HA .23
82 PHE HZ -1.42
83 ALA HN .22
83 ALA HA .61
83 ALA HB1 .12
83 ALA HB2 .12
83 ALA HB3 .12
85 ILE HN -.52
85 ILE HA -.47
85 ILE HB -.75
85 ILE HG21 -.57
85 ILE HG22 -.57
85 ILE HG23 -.57
85 ILE HD11 -1.30
85 ILE HD12 -1.30
85 ILE HD13 -1.30
86 LYS+ HN -.27
86 LYS+ HA -.17
87 LYS+ HN -.27
87 LYS+ HA -.24
88 LYS+ HN -.16
88 LYS+ HA -.27
89 THR HN -.19
89 THR HA -.23
89 THR HB -.22
89 THR HG21 -.19
89 THR HG22 -.19
89 THR HG23 -.19
90 GLU- HN -.34
90 GLU- HA -.35
91 ARG+ HN -.43
91 ARG+ HA -.76
92 GLU- HN -.39
92 GLU- HA -.40
93 ASP- HN -.32
93 ASP- HA -.31
94 LEU HN -.53
94 LEU HA -.58
94 LEU HG -1.30
95 ILE HN -.64
95 ILE HA -.72
95 ILE HB -.52
95 ILE HG21 -.82
95 ILE HG22 -.82
95 ILE HG23 -.82
95 ILE HD11 -.79
95 ILE HD12 -.79
95 ILE HD13 -.79
96 ALA HN -.39
96 ALA HA -.23
96 ALA HB1 -.26
96 ALA HB2 -.26
96 ALA HB3 -.26
97 TYR HN -.32
97 TYR HA -.17
98 LEU HN -.43
98 LEU HA -.15
98 LEU HG -.63
99 LYS+ HN -.24
99 LYS+ HA -.29
100 LYS+ HN -.14
101 ALA HN -.05
101 ALA HA .10
101 ALA HB1 .15
101 ALA HB2 .15
101 ALA HB3 .15
102 THR HN -.06
102 THR HA .33
102 THR HG21 .20
102 THR HG22 .20
102 THR HG23 .20
103 ASN HN .02
103 ASN HA .06
104 GLU- HN .12
104 GLU- HA .05
134 LTNS PCN